Determination of Fate of Polycyclic Aromatic Hydrocarbons (PAHs) in Water, Air, Soil/Sediment at Serokai River, a Tributary of Kinta River, Perak Darul Ridzuan

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ABSTRACT

The main objective of this project is to perform a study on the existence of 7 Carcinogenic Polycyclic Aromatic Hydrocarbon (PAHs) in 3 major environmental media primarily consists of water, air soil/sediment. To achieve the primary objective, several procedures are applied to perform analysis of water, soil/sediment and air samples to proof on the existence and study the distribution and interaction of the 7 Carcinogenic PAHs in 3 major environmental media stated and to focus on the application of software-generated model to predict and demonstrate the distribution and interaction of the 7 Carcinogenic PAHs which are harmful to human health and comes from multiple combustion of carbon-containing fuels sources.

The location that was been chosen to conduct the project is at Serokai River located near Station 18, Ipoh which is one of the tributaries of Kinta River. The reason why this location was been chosen is that, although several studies have been conducted to study the behaviour and interaction of Carcinogenic PAHs in a river flow, there were no studies on the of PAHs behaviour and interaction that has been conducted yet at Serokai River. Besides that, it is identified that Serokai River has a pathway primarily through potential source of Carcinogenic PAHs which comes from timber and metal industrial area, as well as workshops, and it is classified as class III (slightly polluted) for water quality index (WQI) by the Department of Environment of Malaysia.

After the analysis from Gas Chromatography-Mass Spectrometry are obtained, the fate of PAHs are studied by using a multi-segment version of spatial variability and software-generated simulation for the interaction of PAHs named the Quantitative Water Air Sediment Interaction or QWASI model as the medium to study the PAHs compounds in the river flow in terms of their interaction and distribution in the environmental media, the software has the ability to provide an efficient way to conduct the project and can provide useful predictions on the distribution of the compounds in the environmental media.

1 INTRODUCTION

1.1 Project Background

As the world is moving forward and progressively fast, it has brought a significant impact for most of the sectors including major types of sector such as industrial, transportation, housing sectors, plantation as well as petroleum sector. It is explicitly can be seen that vast amount of multiple types of harmful and life-threatening chemicals that have been produced and are thrown away irresponsibly especially when it comes to urban areas where human populations are high. Urbanization, inevitable consequences of rapid economic development, is a multi-dimensional process with complicated outcomes (Zhu *et al*., 2011), such as increased domestic waste discharge (Wang *et al*,. 2007), and water and air pollution (Cheung *et al*,. 2003; Wang *et al*,. 2007,2011a; Pan *et al*,. 2012; Zhang *et al*,. 2012) Several environmental studies have proved the presence of most types of organics and chemical compounds that can be detected in a detectable amount, particularly at hot spot area where most of the compounds are dumped, that is the river. In addition to that, not only these compounds are released into the river and are flown away by the water, these compounds also possessed several characteristics which enabled them to change dynamically according to the environmental conditions and can be transported by several types of environmental media.

One of the harmful compounds classified as organic compound that are generated and discharged into the environment is Polycyclic Aromatic Hydrocarbon (PAHs). PAHs, also known as Polyaromatic Hydrocarbon is a type of hydrocarbon which comprises of carbon and hydrogen and it consists of ring-type structure known as aromatic rings. PAHs are known to enter the aquatic environments through industrial and urban discharges, petroleum spills, fossil fuel combustion, and atmospheric sedimentation (Latimer *et al*,.1990; Simck *et al*,.1996). In general, PAHs sourced from the combustion of carbon-containing ‘fuels’. Several examples of Polycyclic Aromatic Hydrocarbons (PAHs) that are discovered such as Anthracene, Phenanthrene, Tetracene, Chrysene, Triphenylene, Pyrene, Pentacene, Benzo[a]pyrene, Corannulene, Benzo[ghi]perylene, Coronene, and Ovalene. Sixteen un-substitute PAHs, some of which are considered as being possible or probable human carcinogens, have been listed by the US Environmental Protection Agency as priority pollutants, hence their distribution in the environment and potential human health risks have become the focus of much attention (Manoli *et al*., 2000; Witt, 2000). In addition to that, seven types of Polycyclic Aromatic Hydrocarbon (PAHs) has critically been identified as carcinogenic, a substance identified that can cause cancer and it is considered as a type of pollutant which exhibits a potential of being harmful to the environment as well as to human health.

The project covered a studies on the interaction of 7 Carcinogenic Polycyclic Aromatic Hydrocarbon (PAHs) in the river water flow and to perform an analysis on the interaction of the 7 identified PAHs compounds via three environmental media primarily consists of water, air, soil/sediment and to focus on the development of software-generated model to identify and demonstrate the prediction of distribution and interaction of the 7 Carcinogenic Polycyclic Aromatic Hydrocarbon (PAHs) organic compounds in the four major environmental media stated.

The location that has been chosen to conduct this project is at Serokai River, one of tributaries of Kinta River. The reason why this location is chosen is that, although several studies have been conducted to study the behaviour and interaction of PAHs in river flow, but there were no studies on the of PAHs behaviour and interaction that has been conducted yet at Serokai River. Besides that, it is identified that Serokai River has a pathway primarily through timber and metal industrial area, a potential source of Carcinogenic PAHs, as well as workshops, and the river is classified as classified as class III (slightly polluted) for water quality index (WQI) by the Department of Environment of Malaysia.

By using a multi-segment version of spatial variability and software-generated simulation for the interaction of PAHs, such as the Quantitative Water Air Sediment Interaction or QWASI model as the medium to study the compounds in the river flow in terms of their interaction and distribution in the environmental media, the model has the ability to provides an efficient way to conduct the project and also can provide a useful predictions on the fate of the chemicals and the distribution of the chemicals in the environmental media especially on the water flow surface.

Polycyclic Aromatic Hydrocarbon (PAHs) are a widespread environmental contaminants which have been extensively studied due to their toxicity, carcinogenicity, and mutagenicity (White,1986; Wang *et al*,.2007).It is clearly shown that how essential it is to conduct a detail investigation and to have a deeper understanding of the 7 Carcinogenic PAHs, the way to control and maintaining lower level of carcinogenic PAHs in the environment, and to focus on the transportation, interaction and the dynamic behaviour of the PAHs in 3 major environmental media including water, air, soil/sediment. In addition to that, the distribution of PAHs among these phases is primarily controlled by their physical and chemical properties, such as solubility, vapour pressure, and sorption coefficient, as well as the characteristics of each phase (Readman et al. 1984; Zhou *et al*. 1999). A mathematical model or software is one or the way to determine the fate of Polycyclic Aromatic Hydrocarbon (PAH) theoretically besides using sampling analysis method, even though the nature of the environment is complex to be understood.

1.2 Problem Statement

PAHs primarily can be found in soil and sediment as compared to air and water and sourced mainly from combustion of carbon-containing 'fuels' such as wood, diesel or any oily substances and small portion from cigarette smoke. In addition to that, PAHs has a characteristic called lipophilic which this compound has the ability to react easily with oil compared to water.

An amount of concentration of the Polycyclic Aromatic Hydrocarbons (PAHs) and the fate of this compound that has been transported by these four major environmental media mainly water, air, soil and sediment and how many percentages of Polycyclic Aromatic Hydrocarbons (PAHs) is absorbed and transformed through these 3 major environmental media are very crucial to be understood and studied.

These compounds are highly persistent, toxic, and widespread environmental pollutants, and these reasons they are of major concern (Wang *et al*,.2009). Many Polycyclic Aromatic Hydrocarbons (PAHs) are considered to be mutagenic, or carcinogenic and believed to cause health problems, for example cataracts, kidney and liver damage and jaundice (Dong and Lee, 2009; Long *et al*., 2013; Su *et al*., 1998). As a measure, is vital as to prevent the Polycyclic Aromatic Hydrocarbons (PAHs) from contaminating the environment in many ways especially in the surface waters and to prevent it from compromising the human health.

Besides that, PAHs can be classified as being non-toxic to extremely toxic and it depends on the type of ring structure it possessed and 7 of the PAHs are also classified as possible human carcinogenic.

To mitigate the problems, there are numbers of approaches that can be applied to study the fate of Polycyclic Aromatic Hydrocarbon (PAHs) in the stated 3 major environmental media as to control the spreading of the pollutant. Besides performing field assessment, studies on PAHs are done by software simulation as this method is the most time-saving, less cost and less workforce required because it can generate an instant and clear simulation and prediction of the Polycyclic Aromatic Hydrocarbon (PAHs) distribution and reaction in water, air, soil/sediment, by identifying the correct inputs and useful parameters within a period of 1 year.

1.3 Objectives

The main objective of this study is to investigate the fate of 7 Carcinogenic Polycyclic Aromatic Hydrocarbons (PAHs) in river flow and analyse the distribution and interaction of the compounds via four major environmental media which are water, air, soil and sediments.

In order to achieve the targeted primary objective above, the following methods will be applied for this project:

- To perform experimental procedures to test the water samples for the presence of PAHs by applying Gas Chromatography-Mass Spectrometry (GC-MS) methods.

- To develop a software-generated model using a multi-segment version of spatial variability called QWASI to generate a prediction simulation of the interaction of Polycyclic Aromatic Hydrocarbons (PAH) in river flow through the four major environmental media mainly water, air soil/sediment.

1.4 Scope of Project

The scope of this project is to perform an investigation on the behaviour and interaction of Polycyclic Aromatic Hydrocarbons (PAHs) in the river flow and to analyse the distribution of the PAHs compounds via four environmental media primarily consists of water, air, soil and sediment and to focus on the application and development of mathematical model to identify and demonstrate the prediction of distribution of the Polycyclic Aromatic Hydrocarbons (PAHs) compounds in the four major environmental media stated.

Besides that, this is also involved the experimental methods to detect the presence of PAHs in water samples by applying GC-MS methods.

The location that has been chosen to conduct the project is at Serokai River, one of the tributaries of Kinta River, Perak Darul Ridzuan. The reason why this location is chosen is that it is identified that Sungai Serokai has a pathway primarily through residential, industrial, as well as workshops, it is classified as class III (slightly polluted) for Water Quality Index (WQI) by the Department of Environment of Malaysia and the river is suspected to be the having sources of PAHs which might be present in the river flow.

Furthermore, numbers of data that needs to be identified, study and analyse including the detail of the parameters of the Serokai River, the physical and chemical properties of the types of Polycyclic Aromatic Hydrocarbons, and also the calculations and formulae involved in the development of the mathematical model. At the end of the project, both the data collected from the river obtained from the field assessment and the data generated from the mathematical model will be compared and the validity will be confirmed.

2. LITERATURE REVIEW

Various studies have been conducted to investigate the fate of PAHs and how the distribution and interaction of the compounds in the environment via multiple environmental media. Along with the multiple versions of the studies on the fate of PAHs in the environmental media, there are various environmental conditions where the PAHs originated from and also multiple techniques to approach and procedures followed on investigating and studying how much the compounds are distributed and how it interacts via the environmental media.

Below are the comparisons of research papers involving the fate of PAHs and the distribution of the compounds in the environment via various environmental media. The research papers are compared based on the main issue raised and what are the writer's approaches towards the PAHs in each environmental media involved.

2.1 Research Papers on the Main Issues Raised

PAHs can come from multiple sources and there are various ways on how PAHs can affect the surrounding environment. Below are the comparison between research papers in terms of main issues raised regarding the PAHs existence, it sources and how does it affect the environment.

Table 1: Comparison of Research Papers with Reports on PAHs

RESEARCH PAPERS	REPORTS ON PAHs
Polycyclic Aromatic Hydrocarbons in Water, Sediment, Soil and Plants of the Aojiang River Waterway in Wenzhou, China Author: Jianwang Li *et al*. (2009)	The local water system (Aojiang River Watershed) has been heavily polluted by the leather industry which involved processed raw leather materials that is the main source of Polycyclic Aromatic Hydrocarbons (PAHs).
Occurrence of Polycyclic Aromatic Hydrocarbon in Soan River, Pakistan: Insights into Distribution, Composition, Sources and Ecological Risk Assessment Author: Faiqa Aziz *et al*. (2014)	The Soan River affected due to its proximity to densely inhabited areas and to the anthropogenic activities along the river. Besides that, heavy density vehicular emissions in atmosphere and their dry or wet base deposition in the water.
Distribution and Transportation of Polycyclic Aromatic Hydrocarbons (PAHs) at the Humen river mouth in the Pearl River Delta and Their Influencing Factors Author: Feng Liu *et al*. (2014)	The high population densities and heavy industrial development have caused the discharge of various chemicals into the river and one of the chemicals is Polycyclic Aromatic Hydrocarbons (PAHs).
A Multimedia Fate Model to Evaluate the Fate of	The Songhua River is a main receptor of Polycyclic Aromatic Hydrocarbons (PAHs) discharged due to

PAHs in Songhua River, China Author: Ce Wang *et al*. (2012)	the establishment of chemical plants and from burning resources located along the riverside.

2.2 Research Papers on the Approaches Taken.

There are several methods of dealing with PAHs from contaminating the environment by understanding their behaviour and characteristics. Below are the comparisons of 4 research papers with respect to the approaches taken towards the understanding of PAHs behaviour in the environment.

Table 2: Comparison of Research Papers with Approaches Taken

RESEARCH PAPERS	APPROACHES TAKEN TOWARDS UNDERSTANDING THE FATE OF PAHs
Polycyclic Aromatic Hydrocarbons in Water, Sediment, Soil and Plants of the Aojiang River Waterway in Wenzhou, China Author: Jianwang Li *et al*. (2009)	The writer only focused on quantifications of the concentrations of 15 types of Polycyclic Aromatic Hydrocarbons (PAHs) excluding acenaphthylene, which are listed as pollutants by the United States EPA in water, soil, sediment and plant samples that are collected from Aojiang River. The method applied by the writer to study the water samples suspected with PAHs is by High-Performance Liquid Chromatography (HP-LC).
Occurrence of Polycyclic Aromatic Hydrocarbon in Soan River, Pakistan: Insights into Distribution, Composition, Sources and Ecological Risk Assessment	The writer focus on investigating the level or the amount of concentrations of Polycyclic Aromatic Hydrocarbons (PAHs), the distribution of the compound, the sources and the health risks which can be caused by the Polycyclic Aromatic Hydrocarbons (PAHs). The writer applied the method of Gas

Author: Faiqa Aziz *et al*. (2014)	Chromatography-Mass Spectrometry to study and investigate the water samples in the river.
Distribution and Transportation of Polycyclic Aromatic Hydrocarbons (PAHs) at the Humen river mouth in the Pearl River Delta and Their Influencing Factors Author: Feng Liu *et al*. (2014)	The writer stated that it is important to evaluate and examine the distribution and know the characteristics of the Polycyclic Aromatic Hydrocarbons (PAHs) along its transportation processes and to understand the factors influencing the processes which are extremely vital in the discovery of the distributional ways of Polycyclic Aromatic Hydrocarbons (PAHs). In this research , the writer performed test on the water samples by applying the method of Gas Chromatography-Mass Spectrometry (GC-MS).
A Multimedia Fate Model to Evaluate the Fate of PAHs in Songhua River, China Author: Ce Wang *et al*. (2012)	The writer apply the mathematical model and illustrated the spatial and temporal distributions (the distribution of Polycyclic Aromatic Hydrocarbons (PAHs) according to space and time) of the Polycyclic Aromatic Hydrocarbons (PAHs) compounds in the environmental media and the results obtained will be used to measure and classify the water quality and chemical emissions. The writer applied the multi-segment version of spatial variability QWASI software and used to generate simulation of interaction of PAHs in the river flow via water, air, sediment/soil.

2.2.1 Polycyclic Aromatic Hydrocarbons in Water, Sediment, Soil and Plants of the Aojiang River Waterway in Wenzhou, China

This research paper was written by Jianwang Li *et al*. (2009) and this paper demonstrated the main issue which the Polycyclic Aromatic Hydrocarbons have polluted the local water system that is the Aojiang River Watershed which the compounds originated from the output of the leather industry which it is involved in the processed of raw leather materials such as the skin, hide and even hair through the practices of degreasing, dyeing, and decomposing of organic matters. Furthermore, the writers also stressed that the leather industry consumes a vast volumes of sulphide and lime which is used for hair fade, degreasing and dyeing of furs.

Then the writers explained on what are the type of approaches taken to investigate and quantified the 15 types of Polycyclic Aromatic Hydrocarbon (PAH) which the writers stated in the research paper excluding one type of PAHs that is Acenaphthylene.

The writers stated that the investigation to determine whether the leather industry is the root source of Polycyclic Aromatic Hydrocarbons (PAHs) in the Aojiang is done by establishing 14 sampling points. Under the section of chemicals, sample collections and preparation, firstly the writers explained on the sample collection from water and what are the tools and equipment applied. It is also explained that certain processes to extract the PAHs from the water samples and the specific procedures involved to further extract and identified the types of PAHs.

Secondly, the writers explained on steps to collect the samples of sediments and soils and how both of the samples are extracted and processed to identify the PAHs in the samples. Lastly, the writers explained how the PAHs were identified from the plant samples through multiple steps where the samples are taken from the leaves of Artemisia Santolina Schrenk.

In this research paper, the writer performed water samples testing by applying the method of High Performance-Liquid Chromatography (HP-LC).

The results of the study are illustrated in the tables and through graphical representations of the individual compositions of the types of PAHs identified in the water, sediment, soil and plant samples. The writers also stated that 12 types of PAHs found in water samples, and all 15 types of Polycyclic Aromatic Hydrocarbons (PAHs) found in the sediment and soil samples with both indicates a similar pattern while the PAHs found on the leaves of Artemisia Santolina Schrenk is higher and possesses carcinogenic characteristics. Lastly the writer concluded that the leather industry contributed towards PAHs pollution in the Aojiang River.

2.2.2 Occurrence of Polycyclic Aromatic Hydrocarbon in Soan River, Pakistan: Insights into Distribution, Composition, Sources and Ecological Risk Assessment

The research paper is written by Faiqa Aziz *et al*. (2014). This research paper explained the issue on the Soan River which is affected due to its closeness to densely populated areas and to the anthropogenic activities along the river. Besides that, the writers also stressed that heavy density vehicular emission in atmosphere and their dry or wet base deposition in the water also contributed towards the root cause of pollution in the Soan River.

The writers focused on investigating the level or the amount of concentrations of PAHs, the distribution of the compound, the sources and the health risks which can be caused by the Polycyclic Aromatic Hydrocarbons (PAHs).

The approaches taken in sampling collection and analysis are discussed in details except the only sampling source taken is from the river water. In this study, 10 sampling points established during summer of the year 2013.

The next step is the water samples undergone filtration, heating processes and specific chemicals processes specified in details to extract the PAHs from the water samples. It is stated that a strict quality control and assurance measures were taken along the processes of sampling and analysis. Among the characterization of the types of samples done were pH, total dissolved, total suspended solids, dissolved oxygen, electrical conductivity and the total organic carbon in the water samples. In this study, the writer performed a method called Gas Chromatography-Mass Spectrometry (GC-MS).

As a result of the study, 17 types of Polycyclic Aromatic Hydrocarbons (PAHs) were identified in the Soan River and the concentrations of each PAHs is tabulated and a graphical comparison is made to compare the level of concentration of PAHs in the Soan River with the river in Iran, Sri Lanka, India, China, USA and etc. The writers also conducted an Ecological Risk Assessment (ERA) by applying Risk Quotients (RQ) to assess the unwanted effects initiated by the environmental pollutant in the ecological system.

It is concluded by the writers that the Soan River is found to be slightly polluted with PAHs. Besides that, it is also found that the discharge of untreated domestic and industrial wastewater, the release of petroleum based products and the combustion of solid waste and wood also contributes largely to the existence of PAHs in the Soan River.

2.2.3 Distribution and Transportation of Polycyclic Aromatic Hydrocarbons (PAHs) at the Humen River mouth in the Pearl River Delta and Their Influencing Factors

This research paper was written by Feng Liu *et al*. (2014) which highlighted the issue on the high population densities and heavy industrial development have caused the discharge of various chemicals into the Humen River and one of the chemicals is the Polycyclic Aromatic Hydrocarbon.

The writer stated that it is important to evaluate and examine the distribution and know the characteristics of the PAHs along its transportation processes and to understand the factors influencing the processes which are extremely vital in the discovery of the distributional ways of PAHs.

In this research, the writers conducted the study by collecting 10 water samples from 10 sampling points at the Humen River by using a stainless-steel submersible pump. It is stated in details by the writers on the specific filtration, chemical and heating processes undergone by the water samples in order to extract the PAHs. In addition, the PAHs in the suspended particulate matter that is freeze-dried and filtered was being extracted by accelerated solvent extraction which complied with EPA-3545A method. The writer performed test on the water samples by applying the method of Gas Chromatography-Mass Spectrometry (GC-MS).

In this research, it is concluded by the writers that more than 62 types of PAHs were discovered from the water samples at the Humen River mouth during tidal cycle in the flood season. It is also concluded that the concentrations of the PAHs during the tidal cycle were higher compared to its concentrations during the same cycle in the dissolved phase. The writers stated that the factors influencing the distribution of PAHs are the flood and ebb tides, the salinity of the water, the concentration and the size of the grain of the suspended particulate matter and also the sources of the PAHs itself.

2.2.4 A Multimedia Fate Model to Evaluate the Fate of PAHs in Songhua River, China

This research paper was written by Ce Wang *et al*. (2012) which the writers focused on the Songhua River which it is a main receptor of Polycyclic Aromatic Hydrocarbons (PAHs) discharged due to the establishment of chemical plants and from burning resources located along the riverside. In this research, the writer stressed on development of multimedia model from the Equilibrium Criterion until the development of multi-segment version of spatial variability called QWASI software

In this research papers, the writers applied a mathematical model along with the field assessment and using the mathematical model, the writers are able to illustrated the spatial and temporal distributions or in other meaning, the distribution of PAHs according to space and time, of the PAHs compounds in the environmental media and the results obtained are used to measure and classify the water quality and chemical emissions.

The writers developed a multimedia fate model based on the modified level 4 Fugacity to demonstrate the dynamic characteristics of the river and practiced the model to evaluate the transport and fate of the compounds via the environmental media.

The next step explained by the writers is that, the model structure is developed with the input data identified such as the physical properties of the river, the physical-chemical properties of PAHs, the Fugacity capacity or Z-values, which is the capacity of a media to receive certain amount of chemical, and the transport parameter or D-values, which explained the transport and formation of organic pollutants among the environmental phases.

Next, the writers stated the input parameters and also the formula for calculations required to develop the mathematical model. The formulas are stated by the writers in detail in the research paper. At the end of the study, the values of the observed data which are obtained from the field assessment are compared with the theoretical data obtained from the mathematical model for validation of the values.

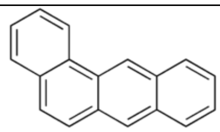
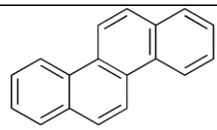
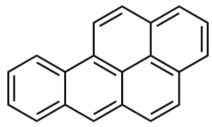
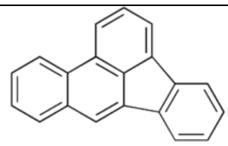
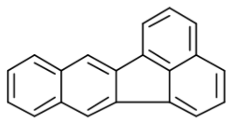
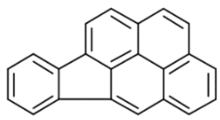
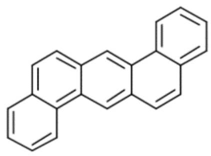
The results of the study were illustrated in the graphical method for each of the environmental media and it is concluded by the writers that the model is able to illustrate the feasibility of evaluating water pollution in Songhua River if the hydrological, geographical and climate conditions are correctly parameterized.

It can be observed that each of the research conducted have a clear problem identification. In terms of reliability of the research papers, it can be stated that the research conducted are reliable as the year the research conducted are not more than 6 years. In addition to that, it is explicitly shown that there are multiple sources of Polycyclic Aromatic Hydrocarbons which can be found in the environment and various methods and approaches are implemented by the researches to investigate the fate of the Polycyclic Aromatic Hydrocarbons (PAHs) in various environmental media. In all the research papers compared above, the writers clearly indicated that the studies applied HPLC, GC-MS as well as QWASI software.

2.3 Types of Polycyclic Aromatic Hydrocarbons (PAHs)

Several examples of Polycyclic Aromatic Hydrocarbons (PAHs) that are discovered such as Anthracene, Phenanthracene, Tetracene, Chrysene, Triphenylene, Pyrene, Pentacene, Benzo[a]pyrene, Corannulene, Benzo[ghi]perylene, Coronene, and Ovalene. 7 out the listed PAHs below are the 7 carcinogenic PAHs. The table below shows the types of 7 Carcinogenic Polycyclic Aromatic Hydrocarbons and their respective molecular structures.

Table 3: 7 Types of Carcinogenic Polycyclic Aromatic Hydrocarbons (PAHs) and Their Respective Molecular Structures

Compound Name	Molecular Structures
Benzo(a)-anthracene	
Chrysene	
Benzo(a)-pyrene	
Benzo(b)-fluoranthene	
Benzo(k)-fluoranthene	
Indeno(1,2,3-cd) pyrene	
Dibenz(a,h)anthracene	

Source: http://en.wikipedia.org/wiki/Polycyclic_aromatic_hydrocarbon

The level of the toxicity of each PAHs is not the same and it depends on the molecular structures of the compounds. The following PAHs lists are the types of PAHs which are listed in the list of Agency for Toxic Substances and Disease Registry and tabulated as below.

Table 4: Types of Polycyclic Aromatic Hydrocarbons (PAHs) Listed in the Agency for Toxic Substances and Disease Registry.

Acenaphthene	Benzo[b]fluoranthene	Dibenz[a,h]anthracene
Acenaphthylene	Benzo[ghi]perylene	Fluoranthene
Anthracene	Benzo[j]fluoranthene	Fluorene
Benz[a]anthracene	Benzo[k]fluoranthene	Indeno[1,2,3-cd]pyrene
Benzo[a]pyrene	Chrysene	phenanthrene
Benzo[e]pyrene	Coronene	Pyrene

Source: http://en.wikipedia.org/wiki/Polycyclic_aromatic_hydrocarbon

2.4 Sources of Polycyclic Aromatic Hydrocarbon (PAH) in Water Stream.

Polycyclic Aromatic Hydrocarbons (PAHs) exhibited a characteristic known as lipophilic where this characteristic gave the organic compounds the ability to mix easily or dissolve in substances such as oils, fats and lipids as compared to water. Furthermore, the ability of dissolving is dependent of the size of the compounds itself. As a result, the larger size of the compounds tends to be less soluble in water and become less volatile.

PAHs is highly related to oil spills. There are several reports of increased cancer incidence in marine animals found within the vicinity of oils spills (Al-Yaakob *et al*., 1994; Colombo *et al*., 2005).

Studies have found that Polycyclic Aromatic Hydrocarbons (PAHs) in the atmosphere are mostly (90% of most Polycyclic Aromatic Hydrocarbons (PAHs) in Earth) in the gas phase (Yan *et al*., 2012). The largest emissions of

PAHs result from industrial processes and other human activities such vehicle exhausts, agricultural burning, residential wood burning, municipal and industrial waste incineration, and hazardous waste sites (WHO Denmark, 2000). Based on the statement, the air act as the main medium to transfer Polycyclic Aromatic Hydrocarbons (PAHs).

Due to that, rainwater may be a primary non-point source of PAHs in the region because both gaseous and particulate of this compounds can be easily scavenged by rainfall (Yan *et al*., 2012).

In our daily food, naphthalene, one of the common PAHs was detected in six of eight samples of human milk (WHO Denmark, 2000). Cooking meat or other food at high temperatures, during grilling or charring, increases the amount of Polycyclic Aromatic Hydrocarbon (PAH) in the food. An experiment done with mice, where 80% of Benzo(a)pyrene was recovered from faeces after 7 days, while a total of 42% was recovered from faeces and urine in rats (WHO Denmark, 2000), suggests that the organic compounds can also be discharged into urban wastewater through human waste.

Furthermore, PAHs may be in groundwater near disposal sites where construction wastes or ashes are buried. Another few sources this organic compounds of include liquid waste discharge of industrial activities, such as primary aluminium and coke production, petrochemical industries, rubber tire and cement manufacturing, bitumen and asphalt industries, wood preservation, commercial heat and power generation and waste incineration (Lee, 2010).

The United States Environmental Protection Agency has classified 7 types of Polycyclic Aromatic Hydrocarbons (PAHs) mainly:

i. benzo[*a*]pyrene,
ii. benz[a]anthracene,
iii. chrysene,
iv. benzo[b]fluoranthene,
v. benzo[k]fluoranthene,

vi. dibenz[a,h]anthracene, and

vii. indeno[1,2,3-cd]pyrene)

All of the above falls under Group B2, probable human carcinogens (US Environmental Protection Agency, 1999). These types of PAHs are the ones to be studied in this project.

2.5 Multimedia Fate Models to Determine the Fate of Polycyclic Aromatic Hydrocarbons (PAHs).

Many multimedia fate models have been developed to analyse environmental fate of chemicals (Lun *et al*., 1998; Mackay and Diamond., 1989; Mackay and Hickie., 2000). The multimedia environmental models have continuously been upgraded from single segment, such as Equilibrium Criterion Model (EQC) (Mackay *et al*., 1996a) to a multi-segment version of spatial variability, such as Quantitative Water Air Sediment Interaction (QWASI) (Warren *et al*., 2002).

This project will apply a fugacity based model Quantitative Water Air Sediment Interaction or QWASI in short. This model was developed by Mackay *et al* (1983) and it is applied to formulate and illustrates the fate of chemicals in the river.

The used of this model is alligned with the scope of this project which is to give emphasis on the investigation of fate of Polycyclic Aromatic Hydrocarbons (PAHs) and the distribution of the compounds in the river flow via four environmental media which are water, air, soil and sediment and to focus on the application and development of mathematical model in order to identify and demonstrate the prediction of distribution of the Polycyclic Aromatic Hydrocarbons (PAHs) in the stated four environmental media.

The QWASI fugacity based model is chosen to be applied for this project as it has the advantages of describing the fate of a chemical in the lake and river system and used to establish the ultimate fate of the contaminants but this model also has the ability to predict the possible recovery times of an air-water-sediment system (El-Shaarawi, 1991).

2.6 Detection Methods of Polycyclic Aromatic Hydrocarbons (PAHs) in Water Samples.

Based on Table 2, the comparison of research papers in terms of approaches taken, there are two main types of methods applied by the both of the research writers, which are:

2.6.1 Gas Chromatography-Mass Spectrometry (GC-MS)

GC-MS is a combination of gas-liquid chromatography with mass spectrometry, which is a method applied to identify different substances in a sample.

Figure 1: GC-MS Instrument

3 METHODOLOGY

3.1 Fugacity Based Model

This project applied a multi-segment version of spatial variability fugacity based model called Quantitative Water Air Sediment Interaction or QWASI in short. This model was developed by Mackay *et al* (1983) and it is applied to formulate and illustrates the fate of chemicals in the river.

This is parallel with the primary objective of this project which is to give emphasis on the investigation of fate of Polycyclic Aromatic Hydrocarbons (PAHs) and the distribution of the compounds in the river flow via four environmental media which are water, air, soil and sediment and to focus on the application and development of mathematical model in order to identify and demonstrate the prediction of distribution of the PAHs in the stated four environmental media.

QWASI fugacity based model is chosen for this project because besides it has the advantages of describing the fate of a chemical in the lake and river system and used to establish the ultimate fate of the contaminants but this model also has the ability to predict the possible recovery times of an air-water-sediment system (El-Shaarawi, 1991).

By using a multi-segment version of spatial variability and software-generated simulation for the interaction of PAHs, such as the Quantitative Water Air Sediment Interaction or QWASI model as the medium to study the compounds in the river flow in terms of their interaction and distribution in the environmental media, the model has the ability to provides an efficient way to conduct the project and also can provide a useful predictions on the fate of the chemicals and the distribution of the chemicals in the environmental media especially on the water flow surface. In addition to that, the results obtained from QWASI model will be supported and the values will be strengthen by field assessment consists of water sampling activities conducted and both of the results are then compared for their integrity towards each other.

3.2 Project Location

Sungai Kinta is one of the main river that is crucial for supplying water to be consumed by highly populated area such as Ipoh, Perak. Kinta River which is 100 kilometres in length that flows from Gunung Korbu at Ulu Kinta, Tanjung Rambutan and ends at Sungai Perak and has a river basin area of 2500 square kilometres.

For conducting this study, Serokai River, has been chosen as the location for field assessment to obtain observed data of the fate of Polycyclic Aromatic Hydrocarbons (PAHs) in the river flow. The river is 3.42 kilometres in length and with an average width of 5 meters. The river is one of the tributaries of Sungai Kinta.

The reason why Serokai River is chosen is that it is identified that Serokai River has a pathway primarily through residential, industrial, as well as workshops, it is classified as class III (slightly polluted) for water quality index (WQI) by the Department of Environment of Malaysia and the river is suspected to be the having sources of PAHs which might be present in the river flow.

Besides that, Serokai River is chosen as the location of project is because it is one of the tributaries which contributed towards the pollution level of Kinta River. Serokai River has a history in oil and grease pollution. River water quality for oil and grease of five main river basins (Bernam, Beruas, Kurau, Perak and Sepetang) in Perak between 2005 to 2009 ranged from 0.5 to 1.00mg/L except for readings at 3.750 mg/L in 2007 and 1.625 mg/L in 2008 at Serokai River (Perak River basin) (Tang, 2011). Below are the images of Serokai River pathway viewed in map view and satellite view.

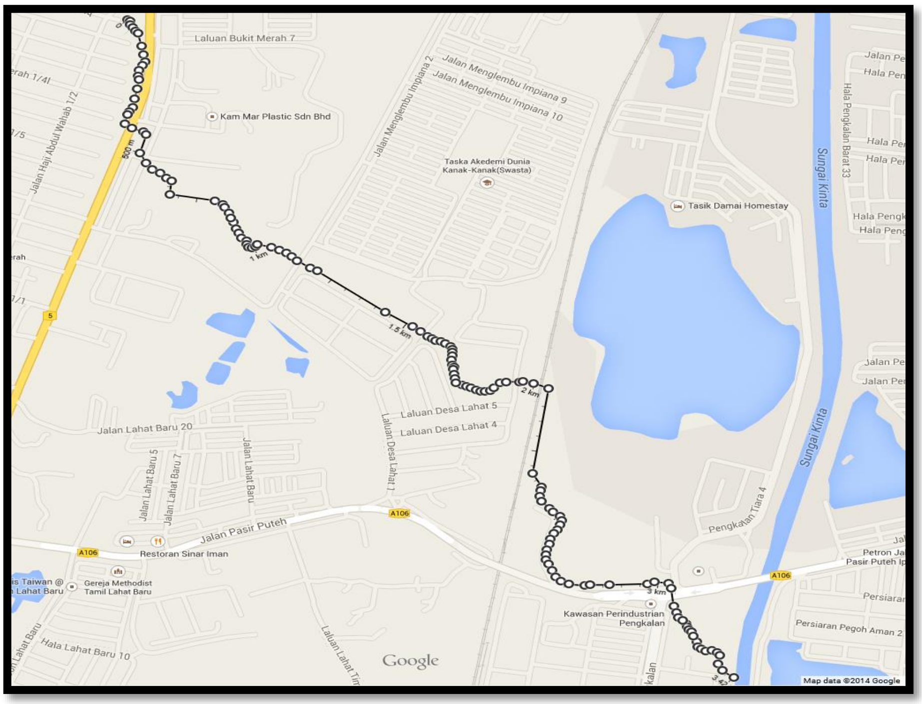


Figure 2: Serokai River pathway in map view

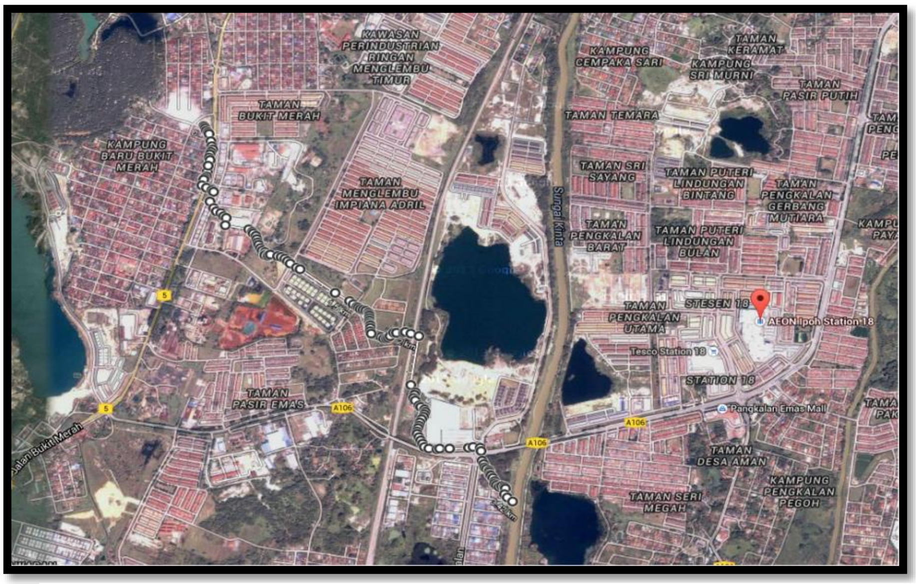


Figure 3: Serokai River pathway in satellite view

3.3 Flow of the Project

The flowchart below is a brief illustration of the flow of the project.

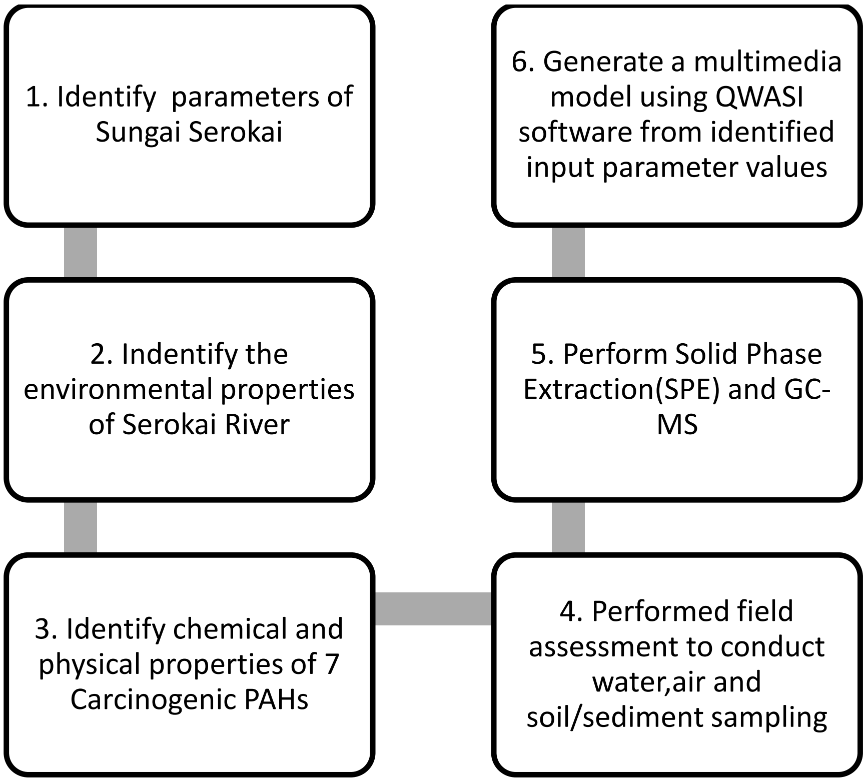


Figure 4: The Flow of the Project

This project consists of two parts, mainly the first part which involved water, air and soil/sediment sampling and the second part of the project which involved the generation of multimedia model using software called QWASI.

3.4 The QWASI Fugacity Based Model: The Required Input Data

The QWASI model requires the user to input parameter values such as the chemical properties of the compound to be studied, the environmental properties of the location of studies as well. In detail, the required input parameters can be seen in APPENDIX 4, 5, 6, 7, 8 and 9.

3.4.1 The Physical Characteristics and Environmental Properties

Firstly, the data required as the input parameters in the model are the physical and environmental properties which are:

i. Length
ii. Depth

iii. Width
iv. Surface area
v. Slope of the river
vi. Bottom roughness
vii. Water flow rates
viii. Concentration of solids in water column, inflow water, aerosol in air and in sediments
ix. Density of solids in water, sediments and aerosol
x. Organic carbon fraction of solids in water column, sediments, inflow water and re-suspended sediment

3.4.2 Determination of the physical and chemical properties of the Polycyclic Aromatic Hydrocarbon (PAHs).

Secondly, the physical-chemical properties of Polycyclic Aromatic Hydrocarbons (PAHs) need to be obtained.
The required physical-chemical properties of Polycyclic Aromatic Hydrocarbon (PAH) include:

i. Melting point
ii. Molecular weight
iii. Water solubility
iv. Enthalpy of Vaporization
v. Henry's Law Constant
vi. Sorption Partition Coefficient for Soil and Sediment
vii. Vapour pressure
viii. Half-life Degradation

3.4.3 Engineering Fieldworks to Determine the Physical and Environmental Properties of Serokai River

The determination of essential geometric properties of Sungai Serokai is performed by calculating:

- Top width
- Bottom width

- Depth
- Wetted area
- Wetted perimeter
- River bed slope
- Bottom roughness

The measurement of top width and the bottom width are illustrated by the Figure below:

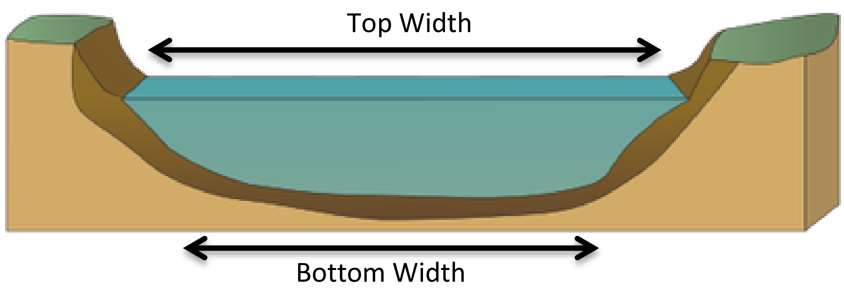


Figure 5: The cross-section of illustration of top width and bottom width of a river

Source: http://ian.umces.edu/imagelibrary/displayimage-topn--114-6199.html

Top width and bottom width is important in determining the flow rates of Serokai River. The flow rate is measured by applying the following methods.

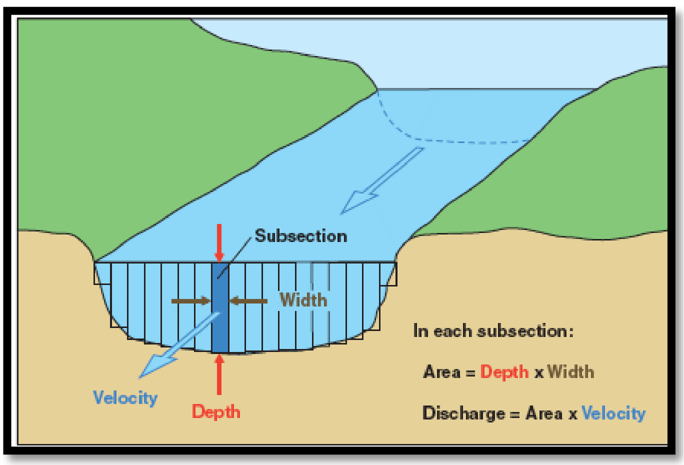


Figure 6: The illustration of cross-sectional area and calculation of flow rates

Source: http://water.usgs.gov/edu/streamflow2.html

The cross-sectional area of the river is divided into multiple rectangular areas and for non-uniform perimeter to calculate the area and flow rates by known velocity of flow that can be calculated as below.

$$Velocity, V = \frac{Distance\ travelled, d\ (m)}{Time\ taken\ (s)}$$

Where in this project, the velocity of water flow is based on the time taken for an established point of the water to travel from point A to point B and the flow rates is calculated by:

$$Flow\ rates\ \left(\frac{m^3}{s}\right)\ or\ Discharge$$
$$= Cross\ sectional\ area\ (m^2)\ x\ Velocity, V\ (\frac{m}{s})$$

An alternative method to measure flow rates is by using flow meter.

The wetted area and wetted perimeter are the cross-sectional area of the water and the length of the soil in contact with the water flow respectively.

The slope of the River will be calculated by applying either the Arithmetic Mean Method of Johstone and Cross (1949) Method. The calculation is shown below.

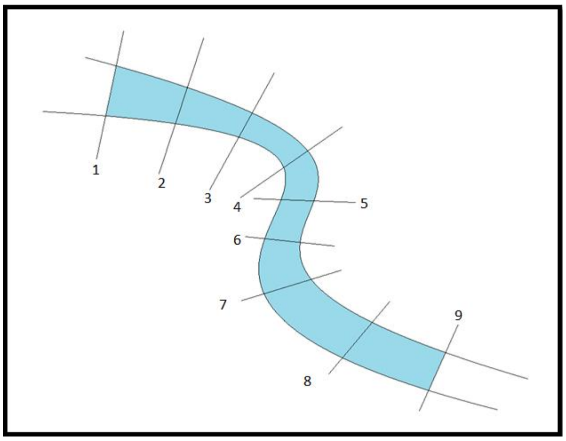


Figure 7: River bed slope calculation

Arithmetic Mean Method:

$$S = \frac{\Delta h}{L}$$

Where:

- S = bed slope
- Delta h = difference in bed elevation along the river from first point at upstream with last point in downstream
- L = Length of the river

Johstone and Cross (1949) Method:

$$S = [\frac{\sum_{i=1}^{N} L_i S_i^{1/2}}{\sum_{i}^{N} L_i}]^2$$

Where:

- S_i = bed slope according to respective segment
- L_i = length of each segment

The value for bottom roughness of the Serokai River is identified by referring to the Manning's Roughness Coefficient table for open channel type by first, identifying the type of bottom surface of Serokai River.

In order to increase reliability of the values obtained from the engineering calculations, a visit to Authorities Offices such as The Department of Irrigation and Drainage of Perak and of Kinta/Batang Padang District is conducted to obtain several data and information regarding the environmental properties and physical properties of Sungai Serokai.

Figure 8: Visit to Department of Irrigation and Drainage of Kinta/Batang Padang District

Figure 9: Meeting with Mr. Taqiuddin Azmy bin Zawawi, Deputy Director for Water Resource Management and Hydrology, Department of Irrigation and Drainage of Perak in Ipoh, Perak Darul Redzuan.

The chemical properties of the 7 Carcinogenic PAHs are obtained as below:

Table 5: Chemical Properties of 7 Carcinogenic PAHs

Compound name	Formula	Mol.wt. (g mo l^{-1})	Vapor pressure at 25 °C (Pa)	Boiling point (°C)	Melting point (°C)	Water solubility (mg/L)	Vapor pressure (mmHg)	Partition coefficient, log K_{OW}	Henry's law constant, H (atm-m3/mol)
Benzo(a)-anthracene	$C_{18}H_{12}$	228.2879	6.52×10^{-7}	438	160.7	0.009	2.8×10^{-8}	5.91	1.22×10^{-6}
Chrysene	$C_{18}H_{12}$	228.29	1.04×10^{-6}	448	254	0.00179	6.3×10^{-7}	5.79	$9.46x10^{-5}$
Benzo(a)-pyrene	$C_{20}H_{12}$	252.31	6.52×10^{-7}	310–312	179–179.3	0.00162	5.6×10^{-9}	6.35	$1.13x10^{-6}$
Benzo(b)-fluoranthene	$C_{20}H_{12}$	252.3093	1.07×10^{-5}	481	168.3	0.0015	0.00125×10^{-7}	5.78	0.051×10^{-5}
Benzo(k)-fluoranthene	$C_{20}H_{12}$	252.31	1.28×10^{-8}	480	215.7	0.0008	-	6.11	$8.29x10^{-7}$
Indeno(1,2,3-cd) pyrene	$C_{22}H_{12}$	276.33068	-	530	163.6	0.00019	10^{-11}–10^{-6}	6.65	$1.60x10^{-6}$
Dibenz(a,h)anthracene	$C_{22}H_{14}$	278.3466	2.80×10^{-9}	524	266	0.00050		6.75	$1.47x10^{-8}$

Source: http://monographs.iarc.fr/ENG/Monographs/vol92/mono92-14.pdf

3.5 The Field Assessment to Obtain Water, Air and Soil/Sediment Samples Data

The procedures for conducting the field assessment are done firstly by establishing the 5 sampling points for water and soil samples with 1 point for 3 samples each, throughout the Serokai River mainly at the point with highly potential sources of PAHs which includes the discharges of heavy industrial area, housing area, and rubbish area. The samples taken consists of 3 water samples using amber glass bottles and 3 soil samples using 100ml glass beaker and steel spoon for each point and then analysed to determine the Total Organic Carbon (TOC), the UV absorption, Chemical Oxygen Demand (COD), and to perform solid phase extraction (SPE) before conducting GC-MS and HPLC. On the other hand, the air samples are taken via air quality device using the glass-fibre filter papers to trap the particle inside air and then extracted via Soxhlet extraction method (SPE) and finally GC-MS machine took part to perform analysis of PAHs existence in the samples. In addition, Amber glass sampling bottles will be used to take the water samples as to ensure the samples are unaffected and the PAHs that are exists in the samples are free from external light.

Figure 10: Amber glass bottle for water sampling

The analysis of the results will be done after all experimental procedures are performed. As for the time being, all the results from the experimental procedures will be recorded since the experiments are still under progress. The flows of the project on the field assessment part are basically illustrated as below.

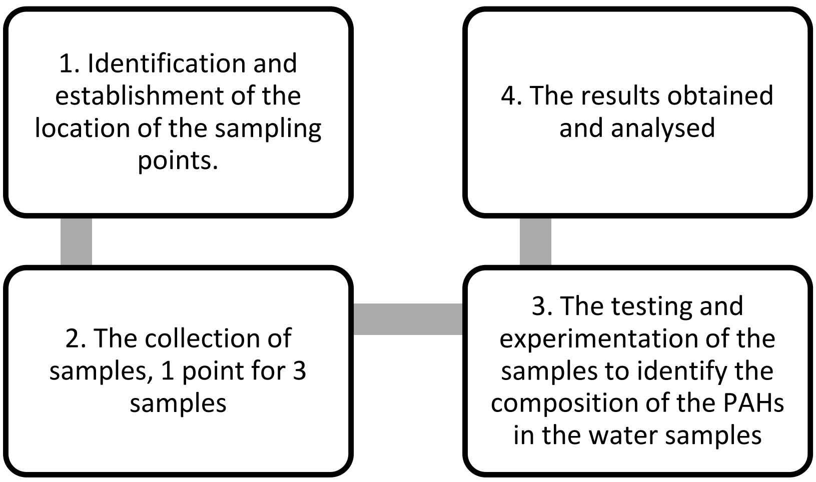


Figure 11: The Flow of the Project on Field Assessment Activity

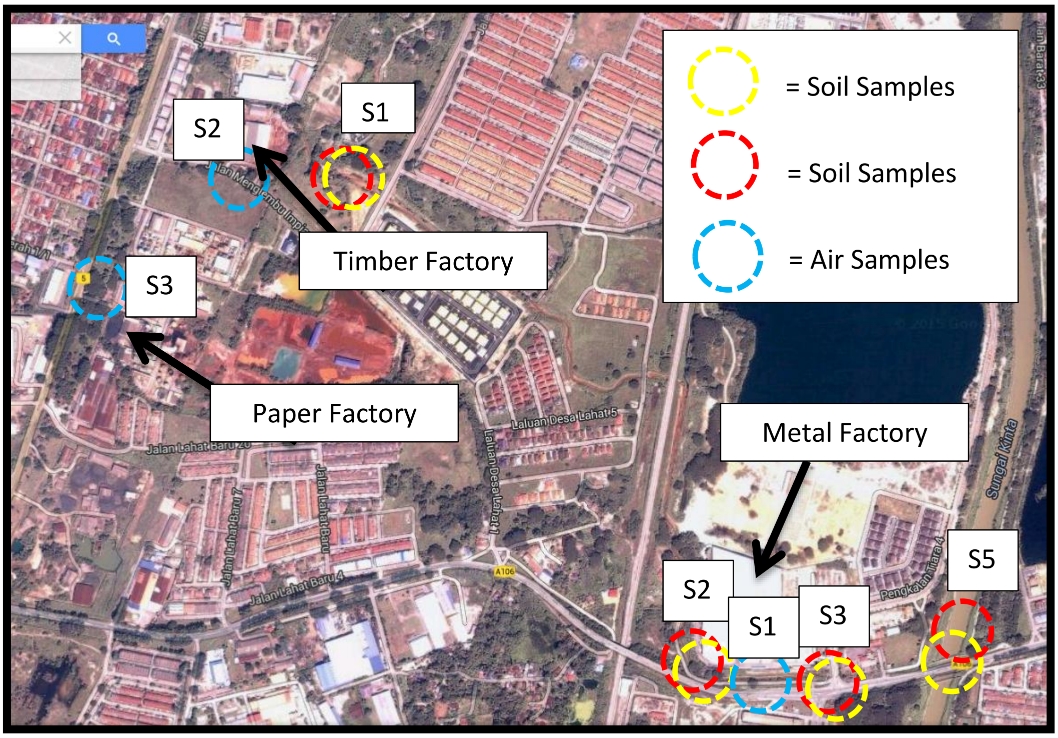


Figure 12: Water, Air and Soil Sampling Points

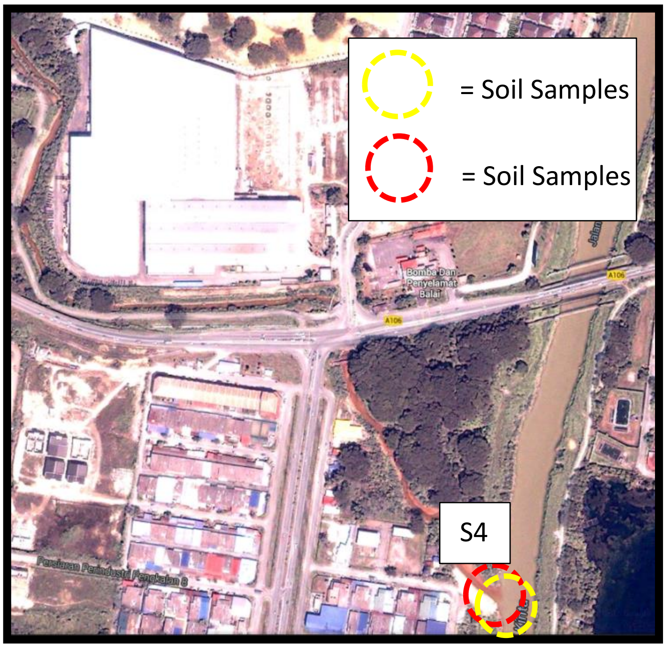


Figure 13: Water and Soil Sampling Points

3.6 Experimental Procedures

Gas chromatography–mass spectrometry (GC-MS) is the experimental method to be applied for determining the type of PAHs that exists in Serokai River.

Before GC-MS is performed it is vital to conduct Solid Phase Extraction (SPE) method which is a method where compounds that are formerly dissolved or trapped in a sample of liquid mixture of known volume are extracted from other types of compounds with respect to their physical and chemical properties.

3.6.1 Solid Phase Extraction for Water Samples

The procedures for solid phase extraction for water samples are:

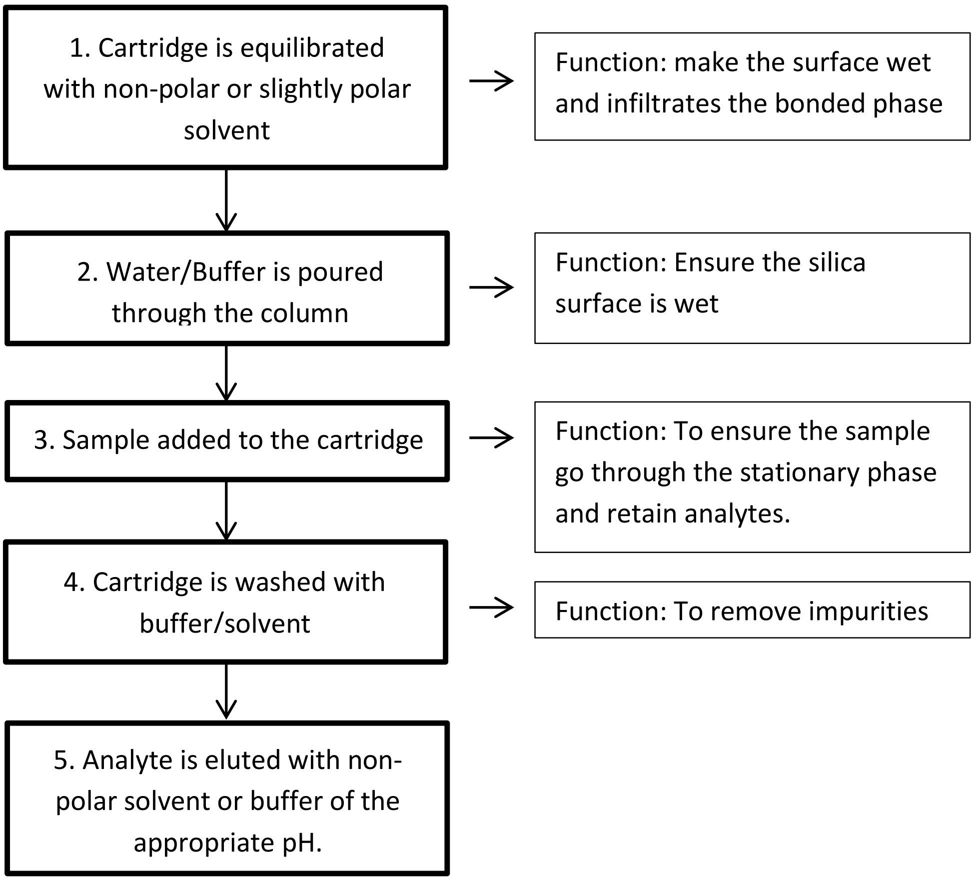


Figure 14: Solid Phase Extraction Methods for Water Samples

A stationary phase of polar functionally bonded silica with short carbons chains frequently makes up the solid phase. The stationary phase will adsorb polar molecules which can be collected with a more polar solvent. After that, the experimental procedures continue with GC-MS method.

Figure 15: Solid Phase Extraction Process for Water Samples

3.6.2 Solid Phase Extraction for Soil Samples

The procedures of extraction for soil samples are done step by step as below. The adopted for the soil extraction procedure is called Ultra-sonication.

The samples are air dried. Next, the samples were screened through sieve with 1mm pore size. 6.0 g of the samples put inside 50 ml beaker. 10 ml acetone, 0.2 g copper powder, 5 g anhydrous sodium sulphate are added. The samples are extracted for 15 minutes at 30 degrees Celsius each in the ultrasonic water bath. The extraction solutions were then centrifuged at 2000 rpm for 15 minutes and the supernatant decanted into 1.5 ml amber vials and stored in the refrigerator until ready for analysis.

Figure 16: Centrifuged Machine

Figure 17: The chemicals required for Soil Extraction which are Anhydrous Sodium Sulphate, Acetone and Copper Powder

3.6.3 Solid Phase Extraction for Air Samples

The procedures for extraction for air samples are adopted as below.

Types of filters used:

1. Glass-Fibre Filters

Pre-treatment of air samples:

Before sampling, filters must be wrapped separately in aluminium foil The filters are baked in the muffle furnace at 450 degrees Celsius for 24 hours.

Extraction of PAHs from Quartz Fibre Filter is done as below.

The glass fibre filter papers are kept in desiccator and then weighed. Extraction of PAHs was performed by Soxhlet extraction method. The glass fibre filter papers were cut in to small pieces with care to avoid loss of dust trapped on it and put in to 30 ml distillation vessel for 6 hrs by using 100 ml cyclohexane in evaporating flask. After extraction, extract was reduced initially with the help of rotary evaporator up to 5 ml and then finally with nitrogen up to 1 ml. If the extract was clear, clean-up was not necessary. The samples are ready for Gas Chromatographic analysis by the method described by Lodge, 1989.

Figure 18: Soxhlet Extraction for Air Sample

3.6.4 UV Test

The test for UV light is performed by using the UV Spectrophotometer. 5 water samples prepared inside the UV Spectrophotometer vials and will be tested for the UV absorption rate and the results of absorption rate are recorded.

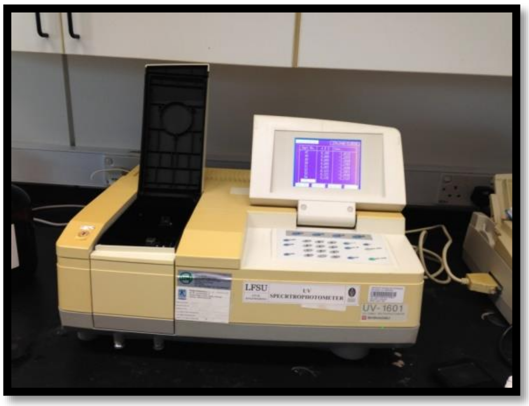


Figure 19: The UV Spectrophotometer

3.6.5 Chemical Oxygen Demand Test

Chemical Oxygen Demand test is a test performed to measure the oxygen consumed chemically by the organic matter. Potassium Dichromate is a chemical used as a source of oxygen and along with high concentrated sulphuric acid. Other reagents used are Mercuric Sulfate, Silver Sulfate and Sulfamic acid. All the chemicals are put inside a vial.

The test for COD will be performed by using the Spectrophotometer and 2mL from 3 samples of 1 sampling points (total of 5 sampling points) are added into the vial with a total of 15 vials for 15 samples. The samples will be left for 2 hours for digestion process at 150 degrees Celsius.

Figure 20: Chemical Oxygen Demand (COD) Test

3.6.6 Total Organic Carbon (TOC) Test

The Total Organic Carbon (TOC) test is performed to measure the amount of carbon that contains in the organic compound. The test is will be done for 4 sampling points of soil samples and 5 sampling points of water samples.

Figure 21: 4 Soil Samples from 4 Sampling Points

Figure 22: 5 Water Samples from 5 Sampling Point

By using TOC devices, 24 soil samples, 12 samples with wool which is TC (Labelled in Blue colour of the devices) and 12 samples without wool which is IC (Labelled in Green colour of the devices), and 5 TOC vials with water samples will be analysed for the content of total organic carbon.

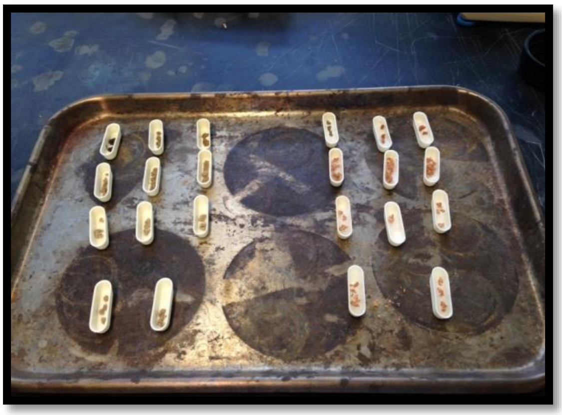


Figure 23: Soil Samples for Total Organic Carbon (TOC) Test

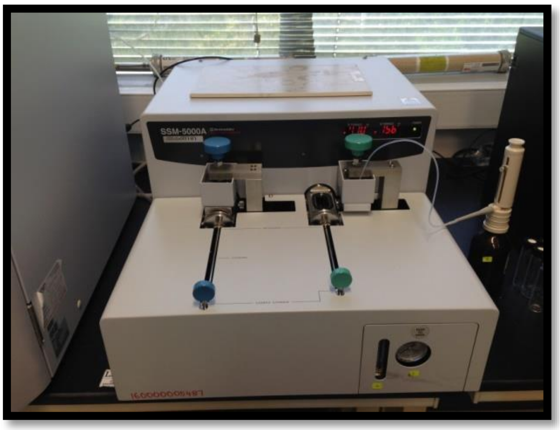


Figure 24: Total Organic Carbon Device for Soil Samples

Figure 25: Total Organic Carbon Device for Water Samples

3.6.7 Gas Chromatography-Mass Spectrometry

GC-MS is a combination of gas-liquid chromatography with mass spectrometer, which is a method applied to identify different substances in a sample.

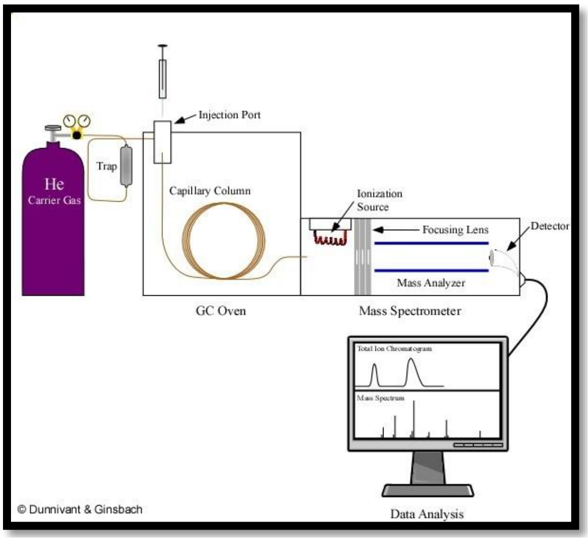


Figure 26: GC-MS flow and Components

Source:
http://texassodiumazidepoisoning.blogspot.com/2013/01/methods-for-gc-ms.html

Gas Chromatography (GC)

1. Injection port

Solvent containing mixtures of molecules is injected into Gas Chromatography part and the sample is transported by inert normally used non-reactive gas, helium, through the instrument. After that, the inject port is heated to a temperature of 300° C and results in changes of the chemicals to become gases states.

2. Oven

The outer part of the GC equipped with an oven**.** The samples in the column is heated in order to transport the molecules over the column. The normal oven temperature is ranging from 40° C to 320° C.

3. Column

The column, which is a thin tube with 30 meters in length, has a special polymer coating on the inside. The chemical mixtures are divided according to their respective volatility and are moved along the column by helium gas. High volatility chemicals tend to travel faster through the column.

Mass Spectrometer (MS)

1. Ion Source

In this process, the molecules are fired with electrons, resulted as a molecular breakdown to small size particles and changed to positively charged particles called as ions. The particles are to be charged in order to pass through the filter.

2. Filter

The ions are then transported through an electromagnetic field which has the ability to filter all the ions according to their respective mass. The range of masses can be controlled. The filter continuously scans through the range of masses as long as the ions keep on coming from the ion source.

3. Detector

A detector has a function to count the number of ions according to specific mass. The data collected is then transferred to the computer and a mass spectrum graph, which is a graph of translated number of ions with different masses that travelled through the filter, is produced. The types of PAHs are identified at this level.

4 RESULTS AND DISCUSSION

The results from extraction methods of water, air and soil/sediment samples and Gas Chromatography-Mass Spectrometry (GC-MS) are tabulated and discussed in Section 4.1, 4.2 and 4.3. The results are divided into three parts consists of results from water, air and soil/sediment samples. The results from QWASI model software simulation also discussed and shown below in Section 4.4 and 4.5. The detail of the statistics calculated by QWASI software can be referred in APPENDIX 4, 5, 6, 7, 8, and 9.

4.1 Results and Discussion from Soil Sample

The results for PAHs concentration (µg/mL) identified in soil samples of the study area is shown in Table 6. Based on the results, it was observed that there are 6 out of 7 carcinogenic PAHs that exists in the Serokai River mainly Benz(a)anthracene, Chrysene, Benzo(k)fluoranthene, Benzo(a)pyrene, indeno(1,2,3-cd)pyrene and dibenz(a,h)anthracene excluding Benzo(b)fluoranthene. It can be seen that the concentrations of the 6 carcinogenic PAHs discovered are focused on soil sample located at S1 which is after timber factory located at coordinate 4°32'58.1"N 101°02'53.7"E near Taman Menglembu Impiana Adril, Ipoh, Perak.

PAHs	S1	S2	S3	S4	S5
Benz(a)anthracene	9.38	0	0	0	0.01
Chrysene	7.15	0.01	0	0	0.01
Benzo(k)Fluoranthene	8.19	0	0	0	0
Benzo(a)pyrene	4.83	0	0	0	0
Indeno(1,2,3-cd)pyrene	58.16	0	0	0	0
Dibenz(a,h)anthracene	62.34	0	0	0	0
2-Methylnaphthalene	0	0	0.02	0	0.01
Anthracene	0	0	0.03	0	0.01
Fluoranthene	0	0	0.01	0	0.20
Acenaphthylene	0	0.02	0	0	0.01
Naphthalene	0	0	0	0.03	0
Benzo(b)fluoranthene	0	0	0	0	0.02

Fluorene	0	0	0	0	0.11

Table 6: Results for PAHs Concentration (μg/mL) Identified in Soil Sample

It is observed at the sampling point that smoke of wood dust from the timber factory exists within airborne particles released from the cutting processing and production area of the factory and being spread into the environment by wind which resulted in the settlement of the wood dust on the surface of the soil located at the riverbank near the factory.

On the other hand, the concentration of the carcinogenic PAHs at Sampling Point S2, S3 and S4 is very low and almost undetectable by Gas Chromatography-Mass Spectrometry (GS-MS). This might be resulted from the significantly less amount of dust being produced and released by Metal factory through the air as observed at the sampling site location and the location of the mixing of Kinta River and Serokai River is located at a distance where dust are unreachable and might already settled on the surface of the soil before reaching the point.

4.2 Results and Discussion from Water Samples

The results for PAHs concentration (μg/mL) identified in water samples of the study area is shown in Table 7. Based on the results, it was observed that there are also 6 out of 7 carcinogenic PAHs that exists in the Serokai River mainly Benz(a)anthracene, Chrysene, Benzo(k)fluoranthene, Benzo(a)pyrene, indeno(1,2,3-cd)pyrene and dibenz(a,h)anthracene excluding Benzo(b)fluoranthene. It can be seen that the concentrations of the 6 carcinogenic PAHs discovered are focused on soil sample located sampling point S1 and S3 which are near wood factory chimney (outlet) after the discharge outlet of metal factory.

PAHs	S1	S2	S3	S4	S5
Benz(a)anthracene	2.13	0	0.74	0	0
Chrysene	2.88	0	1.67	0	0
Benzo(k)Fluoranthene	22.88	4.27	13.77	0	0
Benzo(a)pyrene	14.74	3.95	2.67	0	0
Indeno(1,2,3-cd)pyrene	3.92	0	28	0	0
Dibenz(a,h)anthracene	14.3	12.73	43.07	3.85	0
Anthracene	0.05	0	0	0	0
Acenaphthylene	0	0	0.01	0	0

Table 7: Results for PAHs Concentration (μg/mL) Identified in Water Sample

PAHs are released from coke manufacturing, sintering, iron making, casting, mold poring and cooling and steel making (Nelson et al.,1991). Besides that, in a study outside steel plant on the Swedish Baltic coast for existence of PAHs emitted from steel industry, it is proven at a water surface, annual flux of PAHs in a 10-km^2 area adjacent to the emmission is 290 kg/year (Naf et al.,1992). In addition, a study conducted by Bjorseth et al’s (1985) in Norway, PAH emission from the steel and iron industries represents second major source, accounting for 12 percent of the yearly total-PAHs emission. In this project, the metal factory is located 4°32'26.9"N 101°03'21.7"E just besides Serokai River which related to the production of steel pipe.

Timber factory located at 4°33'01.4"N 101°02'44.4"E along Jalan Menglembu Impiana 21, Menglembu, Perak, is a clear indication that a wood-based industry, which is classified as carbon-containing material is a high potential source of PAHs. This can be proven by a study from Bruschweiler, E. D., et al., (2012) on the generation of Polycyclic Aromatic Hydrocarbons (PAHs) during woodworking operations, carcinogenic PAHs were found from Oak type woods which released Benzo(a)pyrene, Benzo(a)athracene, Benzo(b)fluoranthene, and Benzo(j)fluoranthene.

However, the PAHs concentrations at Sampling Point 4, S4, and Sampling Point 5, S5, are very low and almost undetectable by GC-MS. The possibility of this might happened due to the dilution of PAHs coming into Kinta River and due to a significant increase of size of the Kinta River compared to Serokai River resulted in a drastic reduction of PAHs concentrations. Besides that, it is possible that the PAHs flow in the Serokai River evaporates into the air and settled to an object nearby which is soil/sediment and sand.

4.3 Results and Discussion from Air Samples

The results for PAHs concentration (µg/mL) identified in soil samples of the study area is shown in Table 8 which are Chrysene, Benzo(b)fluoranthene, Benzo(a)pyrene, Indeno(1,2,3-cd)pyrene, and lastly Benzo(k)fluoranthene. All the samples are taken near the factory locations which is located 4°33'01.4"N 101°02'44.4"E along Jalan Menglembu Impiana 21, Menglembu, Perak for timber factory, location of metal factory located 4°32'26.9"N 101°03'21.7"E just besides Serokai River which related to the production of steel pipe and paper factory located near 2-28, Jalan Lahat Baru 1, Taman Pasir Emas, 31500 Ipoh, Perak.

PAHs	S1	S2	S3
Acenaphthalene	0.01	0.01	0.01
Chrysene	0.01	0.01	0.01
Benzo(k)fluoranthene	0.01	0.01	0
Benzo(a)pyrene	0.01	0.01	0
Indeno(1,2,3-cd)pyrene	0	0	0.01
Phenanthrene	0.01	0.01	0.01
Anthracene	0.01	0.01	0.01
Acenaphthylene	0	0	0.01
Benzo(b)fluoranthene	0	0.02	0
Benzo(g,h,i)perylene	0.01	0	0
Fluorene	0.06	0.43	0.56
Fluoranthene	0.44	0.24	0.12
1-Methylnapthalene	0	0.01	0.01

Table 8: Results for PAHs Concentration (µg/mL) Identified in Air Sample

It is observed that the amount of concentration of the PAHs found specifically for 5 carcinogenic PAHs are significantly lower and almost undetectable by GC-MS as compared to the concentration of PAHs found in water and soil sample. However, specific types of PAHs are found to be high compared to others which are Fluoranthene for S1, Fluorene and Fluoranthene for S2 and Fluorene for S3. This is proven based on Fluoranthene and Fluorene where they are found in a plant or facility that makes aluminium based products and uses woods (US Environmental Protection Agency, Agency for Toxic and Disease Registry). Besides that, Fluorene and Fluoranthene are classified by US Environmental Protection Agency under 16 Priority Pollutants.

4.4 QWASI Model Simulation Results

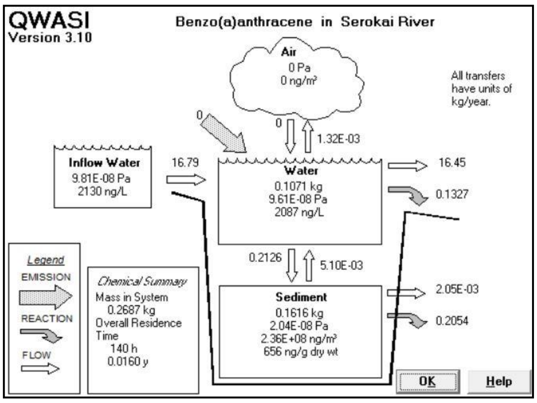


Figure 27: QWASI Model on Benzo(a)anthracene in Water Sample S1

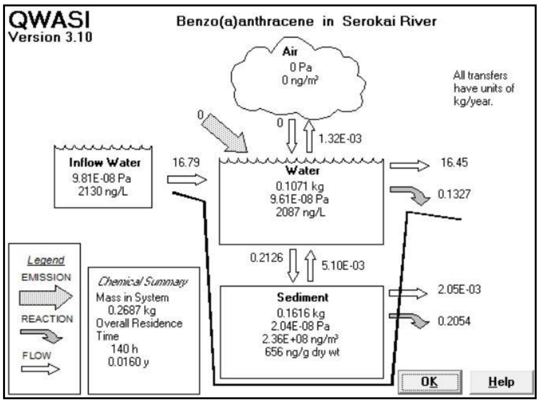


Figure 28: QWASI Model on Benzo(a)anthracene in Water Sample S3

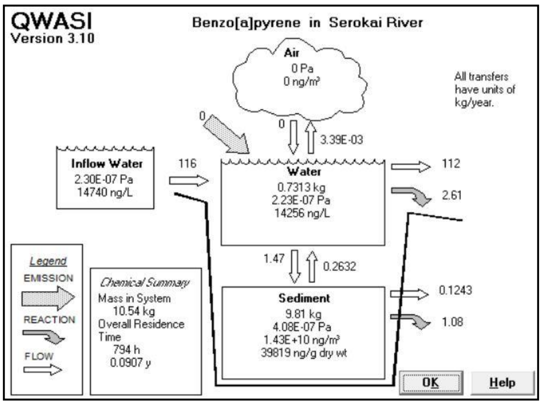


Figure 29: QWASI Model on Benzo(a)pyrene in Water Sample S1

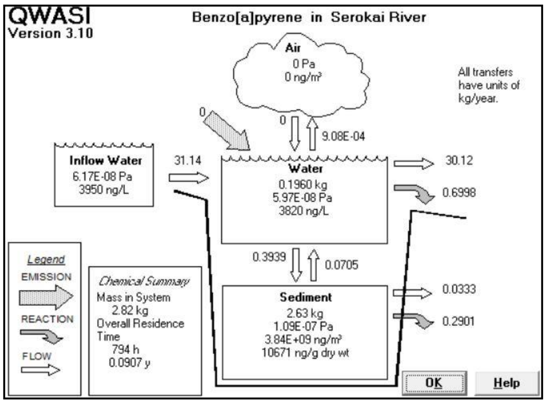


Figure 30: QWASI Model on Benzo(a)pyrene in Water Sample S2

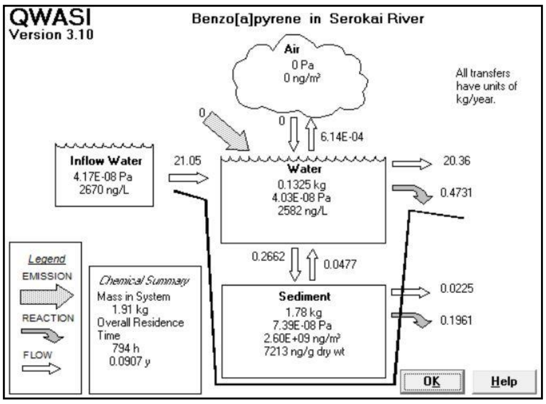


Figure 31: QWASI Model on Benzo(a)pyrene in Water Sample S3

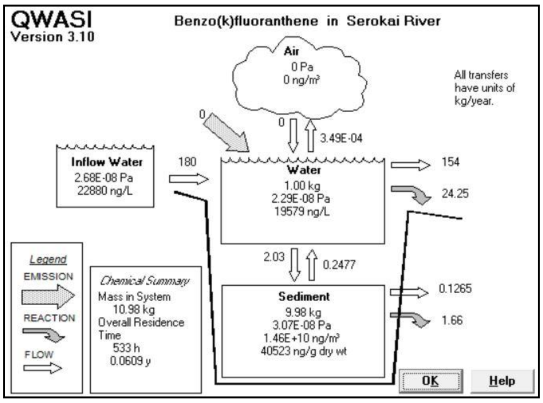


Figure 32: QWASI Model on Benzo(k)fluoranthene in Water Sample S1

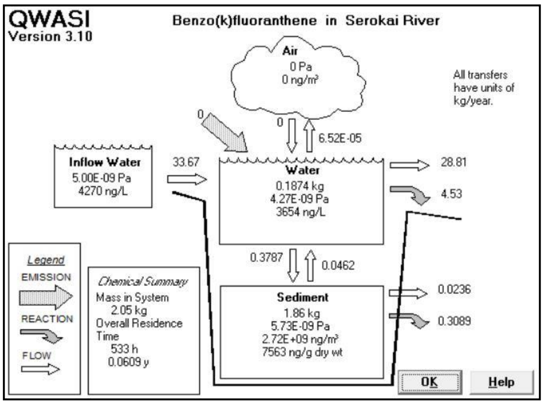


Figure 33: QWASI Model on Benzo(k)fluoranthene in Water Sample S2

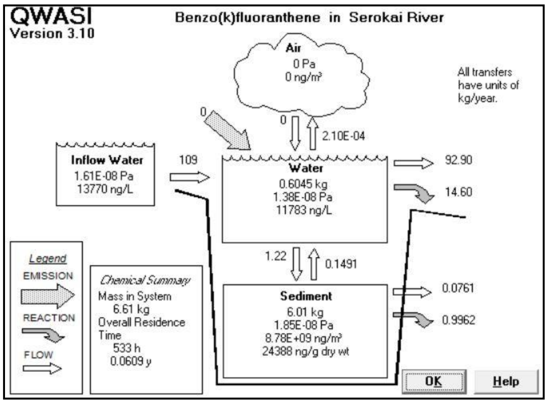


Figure 34: QWASI Model on Benzo(k)fluoranthene in Water Samples S3

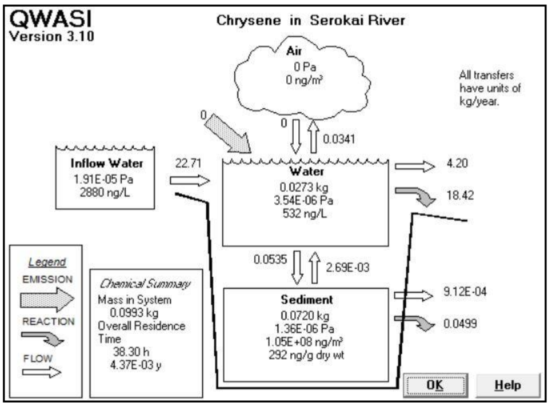


Figure 35: QWASI Model on Chrysene in Water Sample S1

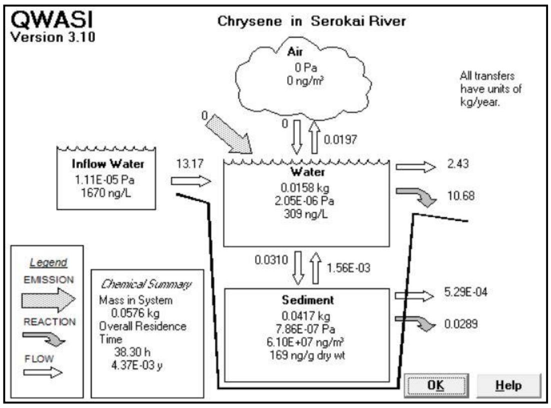


Figure 36: QWASI Model on Chrysene in Water Sample S3

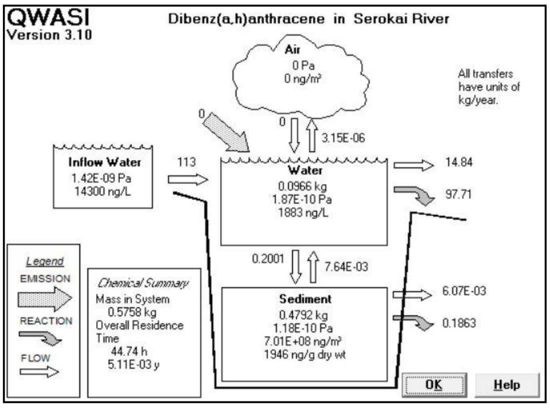


Figure 37: QWASI Model on Dibenz(a,h)anthracene in Water Sample S1

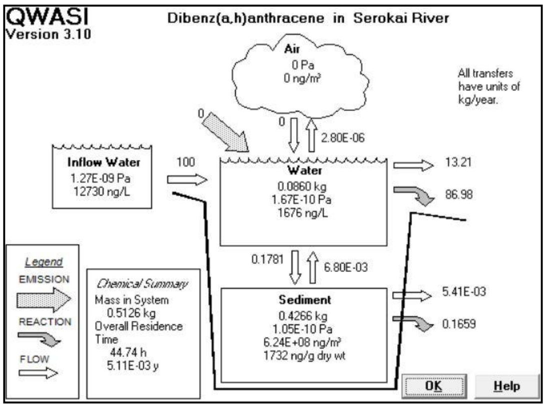


Figure 38: QWASI Model on Dibenz(a,h)anthracene in Water Sample S2

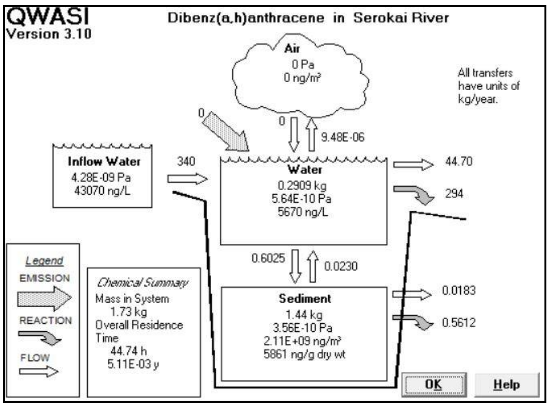


Figure 39: QWASI Model on Dibenz(a,h)anthracene in Water Sample S3

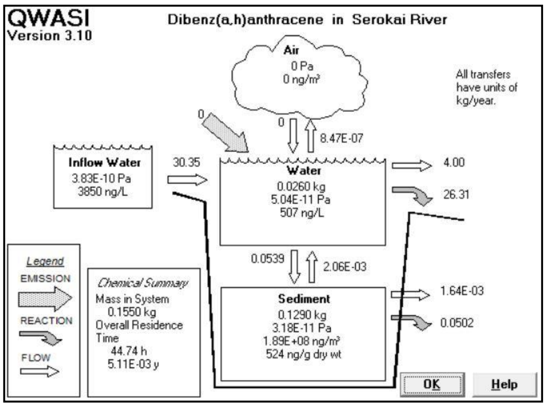


Figure 40: QWASI Model on Dibenz(a,h)anthracene in Water Samples S4

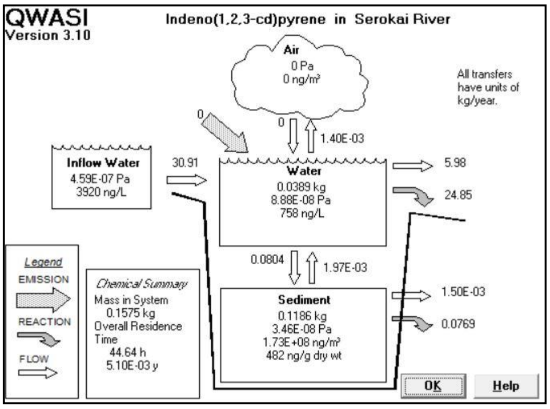


Figure 41: QWASI Model on Indeno(1,2,3-cd)pyrene in Water Sample S1

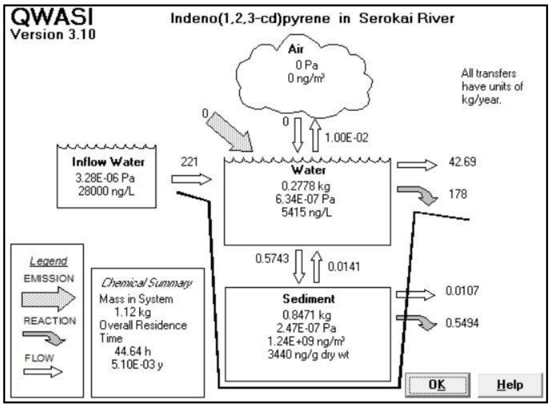


Figure 42: QWASI Model on Indeno(1,2,3-cd)pyrene in Water Sample S3

4.5 QWASI Transfer Rate of PAHs in Water, Air and Soil/Sediment

The results for carcinogenic PAHs concentration transfer rate in water, air and soil/sediment (kg/year) identified in the samples of the study area at Serokai River are shown in Table 9 below.

Carcinogenic PAHs	**Fate of Carcinogenic PAHs**			
	Inflow Water ng/mL (kg/year)	Into Air (kg/year)	Into Soil/Sediment (kg/year)	Outflow (kg/year)
Benz(a) anthracene (S1)	2130 (16.79)	0.00132	0.2075	16.45
Benzo(a)pyrene (S1)	14740 (116)	0.00339	1.2068	112
Benzo(k) Fluoranthene (S1)	22880 (180)	0.000349	1.7823	154
Chrysene (S1)	2880 (22.71)	0.0341	0.05081	4.20
Dibenz(a,h) Anthracene (S3)	43070 (340)	0.00000948	0.5795	44.70
Indeno(1,2,3-cd) pyrene	28800 (221)	0.0120	0.05602	42.69

Table 9: Transfer Rate of carcinogenic PAHs (kg/year) in water, air and soil/sediment

The fate of Benzo(a)anthracene from Sampling Point S1 as shown in Figure 27 (Section 4.4), expressed by the QWASI model is summarized in Table 9. The input of the compound comes from the inflow water. Based on the study and experiment, it was detected in inflow water that the concentration of Benz(a)anthracene is 2130 ng/mL which calculated in the model as 16.79 kg/year. It is observed that 0.00132 kg/year is loss by water into air transfer, 0.2075 kg/year is loss into soil and sediment and 16.45kg/year will be loss in the outflow.

Table 9 also shows that the fate of highest concentration of Benzo(a)pyrene at Sampling Point S1 indicated in Figure 29 (Section 4.4). The compound which was detected in inflow water by experimentation has an amount of 14740 ng/mL and was calculated by QWASI model as being 116kg/year, will be loss into air from water flow amounting 0.00339 kg/year, and 1.7823 kg/year will be transferred into soil and sediment while 112 kg/year will escaped into the outflow.

Besides that, it is shown that the fate of highest concentration of Benzo(k)fluoranthene detected at Sampling Point S1 is 22880 ng/mL which was translated as being 180 kg/L in inflow water will be loss from inflow water into air amounting 0.000349 kg/year, while 1.7823 kg/year is absorbed into soil and sediment. 154kg/year will flow into the outflow. The model simulation is indicated in Figure 32 (Section 4.4).

Figure 35 (Section 4.4) indicated the transfer rate of Chrysene at Sampling Point S1. It is observed also that the fate of Chrysene shown in table 9 initially has a concentration of 2880 ng/L or 22.71 kg/year in inflow water as calculated by QWASI, 0.0341 kg/year will be transferred into air, while 0.05081kg/year is transferred from inflow water into soil and sediment. 4.20 kg/year will escape in the outflow.

On the other hand, the fate of Dibens(a,h)anthracene is simulated by the model and indicated in Figure 39 (Section 4.4). The fate of highest concentration of Dibenz(a,h)anthracene which was detected at Sampling Point S1 by experimentation methods initially has a concentration of 43070 ng/L or calculated by QWASI as 340 kg/year. The compound, as simulated by the model calculated that 0.00000948 kg/year will be loss into air from water inflow, 0.5795 kg/year will be transferred into soil and sediment while the remaining 44.70 kg/year will escaped into outflow.

Last but not least, it is observed that the fate of PAHs compound named Indeno(1,2,3-cd)pyrene which was detected by experimentation methods to be 28800 ng/L and calculated by QWASI as 221 kg/year. Based on the results obtained from the model, 0.0120kg/year will be loss from inflow water into air while 0.05602 kg/year will be transferred into soil and sediment and 42.69 kg/year will loss in the outflow. The QWASI model simulation is indicated in Figure 42 (Section 4.4).

5 CONCLUSION

By using the right tools such as the Quantitative Water Air Sediment Interaction or QWASI model as the medium to evaluate the fate of PAHs in the river flow and to study the distribution of the compounds in the environmental media, not only the model provides an efficient way to conduct the project but also to provide a useful predictions on the fate of the chemicals and the distribution of the chemicals in the environmental media.

In addition to that, the results obtained from experimental procedures such as Solid Phase Extraction and GC-MS is supported by QWASI model simulation where the software provides clear figures for the interaction and distribution of targeted Carcinogenic PAHs in the 3 major environmental media which are water, air and soil/sediment.

Last but not least, this project can act as a gateway to control and reduce the amount of chemicals that are resulted from the output of the industrial as well as domestic area at Serokai River where this river is a major source of water consumption and production in the highly populated are especially to a big city namely Ipoh.

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APPENDIX 1

TOTAL ORGANIC CARBON RESULTS FOR WATER SAMPLE

	Type	Analysis	Sample Name	Sample ID	Origin	Results	Status	Date/Time	Vial
1	Unknown	TOC	S1	Untitled	Method	TOC:5.190mg/L TC:30.20mg/L IC: 25.01mg/L	Completed	14/2/2015	1
2	Unknown	TOC	S2	Untitled	Method	TOC:4.110mg/L TC:28.35mg/L IC: 24.24mg/L	Completed	14/2/2015	2
3	Unknown	TOC	S3	Untitled	Method	TOC:5.024mg/L TC:28.72mg/L IC: 23.70mg/L	Completed	14/2/2015	3
4	Unknown	TOC	S4	Untitled	Method	TOC:3.915mg/L TC:22.24mg/L IC: 18.32mg/L	Completed	14/2/2015	4

TOC-Control L Report

PM_TEST_2015_02_17_001.tlx

Instr.Information

Instrument Options TOC/ASI/
Catalyst Regular Sensitivity

Sample

Sample Name: Kinta River Sample
Sample ID: S1
Origin:
Status Completed
Chk. Result

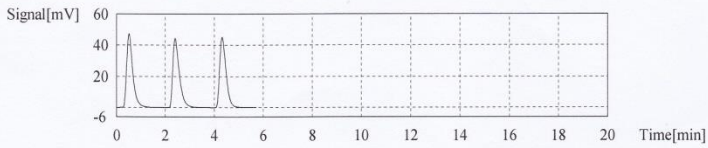
Type	Anal.	Manual Dilution	Result
Unknown	TOC	1.000	TOC:5.190mg/L TC:30.20mg/L IC:25.01mg/L

1. Det

Anal.: TC

No.	Area	Conc.	Inj. Vol.	Aut. Dil.	Ex.	Cal. Curve	Date / Time
1	84.28	32.97mg/L	50uL	1.000	R	TC_STD_1000PPM_170215.2015_02_17_10_57_02.cal	17/2/2015 4:56:18 PM
2	82.51	30.34mg/L	50uL	1.000		TOC_TC_STD_100PPM_170215.2015_02_17_15_21_43.cal	17/2/2015 4:58:23 PM
3	81.76	30.06mg/L	50uL	1.000		TOC_TC_STD_100PPM_170215.2015_02_17_15_21_43.cal	17/2/2015 5:00:28 PM

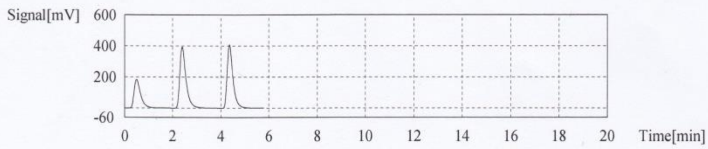
Mean Area 82.14
Mean Conc. 30.20mg/L



Anal.: IC

No.	Area	Conc.	Inj. Vol.	Aut. Dil.	Ex.	Cal. Curve	Date / Time
1	348.2	26.24mg/L	270uL	1.000	R	IC_STD_1000PPM_170215.2015_02_17_11_31_58.cal	17/2/2015 5:06:37 PM
2	704.6	25.07mg/L	540uL	1.000		TOC_IC_STD_100PPM_170215.2015_02_17_15_48_08.cal	17/2/2015 5:12:48 PM
3	701.5	24.95mg/L	540uL	1.000		TOC_IC_STD_100PPM_170215.2015_02_17_15_48_08.cal	17/2/2015 5:15:52 PM

Mean Area 703.0
Mean Conc. 25.01mg/L



Sample

Sample Name: Kinta River Water
Sample ID: S2
Origin:
Status Completed
Chk. Result

1/4 17/2/2015 6:32:28 PM

TOC-Control L Report

PM_TEST_2015_02_17_001.tlx

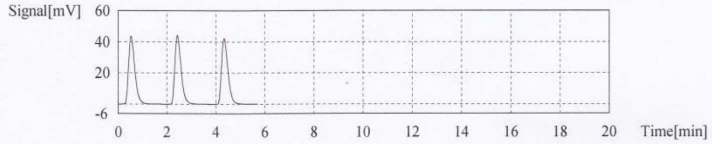
Type	Anal.	Manual Dilution	Result
Unknown	TOC	1.000	TOC:4.110mg/L TC:28.35mg/L IC:24.24mg/L

1. Det

Anal.: TC

No.	Area	Conc.	Inj. Vol.	Aut. Dil.	Ex.	Cal. Curve	Date / Time
1	79.51	31.11mg/L	50uL	1.000	R	TC_STD_1000PPM_170215.2015_02_17_10_57_02.cal	17/2/2015 5:20:58 PM
2	77.63	28.54mg/L	50uL	1.000		TOC_TC_STD_100PPM_170215.2015_02_17_15_21_43.cal	17/2/2015 5:23:03 PM
3	76.57	28.15mg/L	50uL	1.000		TOC_TC_STD_100PPM_170215.2015_02_17_15_21_43.cal	17/2/2015 5:25:08 PM

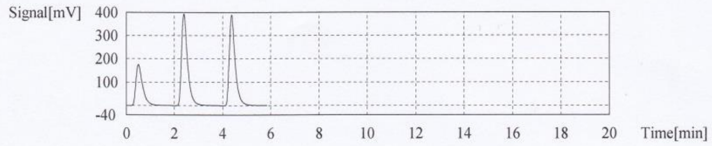
Mean Area 77.10
Mean Conc. 28.35mg/L



Anal.: IC

No.	Area	Conc.	Inj. Vol.	Aut. Dil.	Ex.	Cal. Curve	Date / Time
1	339.5	25.58mg/L	270uL	1.000	R	IC_STD_1000PPM_170215.2015_02_17_11_31_58.cal	17/2/2015 5:31:15 PM
2	683.3	24.31mg/L	540uL	1.000		TOC_IC_STD_100PPM_170215.2015_02_17_15_48_08.cal	17/2/2015 5:37:26 PM
3	679.4	24.17mg/L	540uL	1.000		TOC_IC_STD_100PPM_170215.2015_02_17_15_48_08.cal	17/2/2015 5:40:31 PM

Mean Area 681.4
Mean Conc. 24.24mg/L



Sample

Sample Name: Kinta River Water
Sample ID: S3
Origin:
Status Completed
Chk. Result

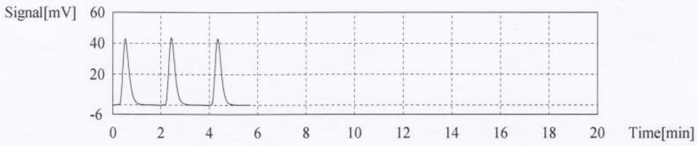
Type	Anal.	Manual Dilution	Result
Unknown	TOC	1.000	TOC:5.024mg/L TC:28.72mg/L IC:23.70mg/L

1. Det

Anal.: TC

No.	Area	Conc.	Inj. Vol.	Aut. Dil.	Ex.	Cal. Curve	Date / Time
1	79.26	31.01mg/L	50uL	1.000	R	TC_STD_1000PPM_170215.2015_02_17_10_57_02.cal	17/2/2015 5:45:37 PM
2	78.65	28.92mg/L	50uL	1.000		TOC_TC_STD_100PPM_170215.2015_02_17_15_21_43.cal	17/2/2015 5:47:42 PM
3	77.57	28.52mg/L	50uL	1.000		TOC_TC_STD_100PPM_170215.2015_02_17_15_21_43.cal	17/2/2015 5:49:47 PM

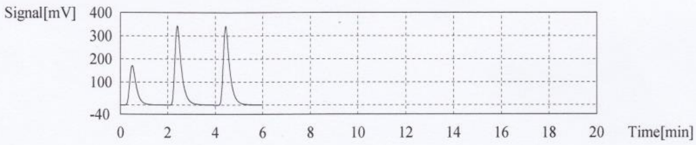
Mean Area 78.11
Mean Conc. 28.72mg/L



Anal.: IC

No.	Area	Conc.	Inj. Vol.	Aut. Dil.	Ex.	Cal. Curve	Date / Time
1	333.0	25.09mg/L	270uL	1.000	R	IC_STD_1000PPM_170215.2015_02_17_11_31_58.cal	17/2/2015 5:55:55 PM
2	667.8	23.76mg/L	540uL	1.000		TOC_IC_STD_100PPM_170215.2015_02_17_15_48_08.cal	17/2/2015 6:02:13 PM
3	664.4	23.63mg/L	540uL	1.000		TOC_IC_STD_100PPM_170215.2015_02_17_15_48_08.cal	17/2/2015 6:05:22 PM

Mean Area 666.1
Mean Conc. 23.70mg/L



Sample

Sample Name: Kinta River Water
Sample ID: S4
Origin:
Status Completed
Chk. Result

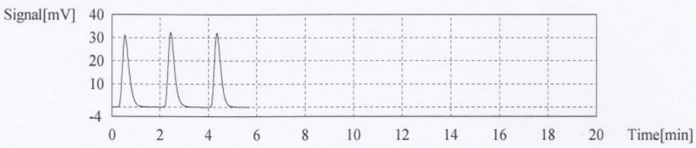
Type	Anal.	Manual Dilution	Result
Unknown	TOC	1.000	TOC:3.915mg/L TC:22.24mg/L IC:18.32mg/L

1. Det

Anal.: TC

No.	Area	Conc.	Inj. Vol.	Aut. Dil.	Ex.	Cal. Curve	Date / Time
1	62.00	24.26mg/L	50uL	1.000	R	TC_STD_1000PPM_170215.2015_02_17_10_57_02.cal	17/2/2015 6:10:28 PM
2	60.91	22.40mg/L	50uL	1.000		TOC_TC_STD_100PPM_170215.2015_02_17_15_21_43.cal	17/2/2015 6:12:37 PM
3	60.06	22.08mg/L	50uL	1.000		TOC_TC_STD_100PPM_170215.2015_02_17_15_21_43.cal	17/2/2015 6:14:42 PM

Mean Area 60.48
Mean Conc. 22.24mg/L



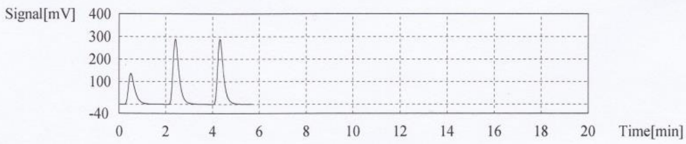
Anal.: IC

TOC-Control L Report

PM_TEST_2015_02_17_001.tlx

No.	Area	Conc.	Inj. Vol.	Aut. Dil.	Ex.	Cal. Curve	Date / Time
1	257.0	19.37mg/L	270uL	1.000	R	IC_STD_1000PPM_170215.2015_02_17_11_31_58.cal	17/2/2015 6:20:51 PM
2	516.5	18.37mg/L	540uL	1.000		TOC_IC_STD_100PPM_170215.2015_02_17_15_48_08.cal	17/2/2015 6:26:59 PM
3	513.7	18.27mg/L	540uL	1.000		TOC_IC_STD_100PPM_170215.2015_02_17_15_48_08.cal	17/2/2015 6:30:00 PM

Mean Area 515.1
Mean Conc. 18.32mg/L



APPENDIX 2

TOTAL ORGANIC CARBON RESULTS FOR SOIL/SEDIMENT SAMPLE

C:\TOC-L\Data\2015_02_14_001_hafiz.tlx

	Type	Analysis	Sample Name	Sample ID	Origin	Result	Notes	Status	Date / Time
1	Unknown	SSM-TOC	S3-1a	Untitled	240114_SS	SSM-TOC:1.619% SSM-TC:1.631% SSM-IC:0.01234%		Completed	14/2/2015 10:55
2	Unknown	SSM-TOC	S3-1b	Untitled	240114_SS	SSM-TOC:0.06783% SSM-TC:0.06783% SSM-IC:0.000		Completed	14/2/2015 11:17
3	Unknown	SSM-TOC	S3-1c	Untitled	240114_SS	SSM-TOC:-0.00724% SSM-TC:0.000% SSM-IC:0.0072		Completed	14/2/2015 11:30
4	Unknown	SSM-TOC	S1-1a	Untitled	240114_SS	SSM-TOC:0.5455% SSM-TC:0.5595% SSM-IC:0.01400		Completed	14/2/2015 12:21
5	Unknown	SSM-TOC	S1-1b	Untitled	240114_SS	SSM-TOC:0.00170% SSM-TC:0.00764% SSM-IC:0.005		Completed	14/2/2015 12:29
6	Unknown	SSM-TOC	S1-1c	Untitled	240114_SS	SSM-TOC:0.7954% SSM-TC:0.7994% SSM-IC:0.00404		Completed	14/2/2015 12:39
7	Unknown	SSM-TOC	S2-1a	Untitled	240114_SS	SSM-TOC:1.295% SSM-TC:1.303% SSM-IC:0.00782%		Completed	14/2/2015 12:49
8	Unknown	SSM-TOC	S2-1b	Untitled	240114_SS	SSM-TOC:1.382% SSM-TC:1.389% SSM-IC:0.00713%		Completed	14/2/2015 12:58
9	Unknown	SSM-TOC	S2-1c	Untitled	240114_SS	SSM-TOC:1.311% SSM-TC:1.317% SSM-IC:0.00610%		Completed	14/2/2015 1:08:
10	Unknown	SSM-TOC	S5-1a	Untitled	240114_SS	SSM-TOC:0.3569% SSM-TC:0.3640% SSM-IC:0.00704		Completed	14/2/2015 1:22:
11	Unknown	SSM-TOC	S5-1b	Untitled	240114_SS	SSM-TOC:0.1571% SSM-TC:0.1736% SSM-IC:0.01644		Completed	14/2/2015 1:34:
12	Unknown	SSM-TOC	S5-1c	Untitled	240114_SS	SSM-TOC:0.2461% SSM-TC:0.2511% SSM-IC:0.00495		Completed	14/2/2015 1:43:
13	Unknown	SSM-TOC	S3-1b(correction)	Untitled	240114_SS	SSM-TOC:1.647% SSM-TC:1.653% SSM-IC:0.00632%		Completed	14/2/2015 1:57:
14	Unknown	SSM-TOC	S3-1c(correction)	Untitled	240114_SS	SSM-TOC:1.870% SSM-TC:1.870% SSM-IC:0.000%		Completed	14/2/2015 2:12:

14/2/2015 2:16:59 PM

1/1

TOC-Control L Report

2015_02_14_001_hafiz.tlx

Instr.Information

Instrument Options	TOC/SSM/
Catalyst	Regular Sensitivity

Sample

Sample Name:	S3-1a
Sample ID:	Untitled
Origin:	240114_SSM TOC method.met
Status	Completed
Chk. Result	

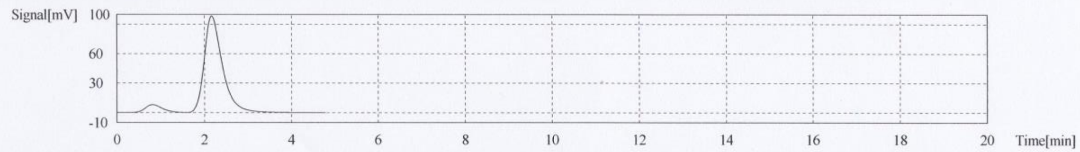
Type	Anal.	Manual Dilution	Density	Result
Unknown	SSM-TOC	1.000	1.000mg/uL	SSM-TOC:1.619% SSM-TC:1.631% SSM-IC:0.01234%

1. Det

Anal.: SSM-TC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	309.9	309.9	2629ug	1.631%	161.2mg	161uL		240114_SSM_TC Std.2014_01_24_10_16_26.cal	14/2/2015 10:48:41 AM

Mean Area	309.9
Mean CNV	309.9
Mean Conc.	1.631%



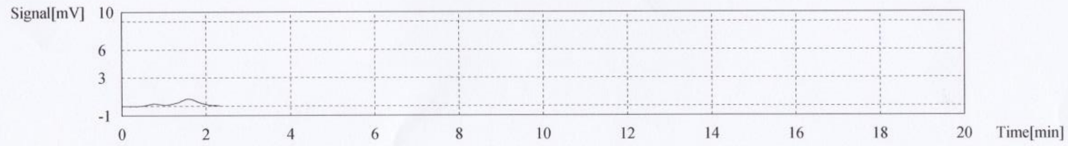
Anal.: SSM-IC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	2.715	2.715	23.76ug	0.01234%	192.5mg	192uL		240114_SSM_IC Std.2014_01_24_11_21_07.cal	14/2/2015 10:55:26 AM

TOC-Control L Report

2015_02_14_001_hafiz.tlx

Mean Area 2.715
Mean CNV 2.715
Mean Conc. 0.01234%



Sample

Sample Name: S3-1b
Sample ID: Untitled
Origin: 240114_SSM TOC method.met
Status Completed
Chk. Result

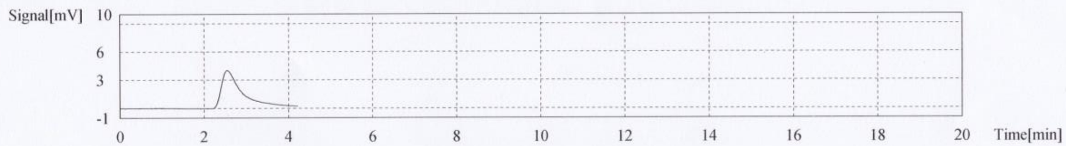
Type	Anal.	Manual Dilution	Density	Result
Unknown	SSM-TOC	1.000	1.000mg/uL	SSM-TOC:0.06783% SSM-TC:0.06783% SSM-IC:0.000%

1. Det

Anal.: SSM-TC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	13.28	13.28	112.7ug	0.06783%	166.1mg	166uL		240114_SSM_TC Std.2014_01_24_10_16_26.cal	14/2/2015 11:06:20 AM

Mean Area 13.28
Mean CNV 13.28
Mean Conc. 0.06783%



Anal.: SSM-IC

2/16

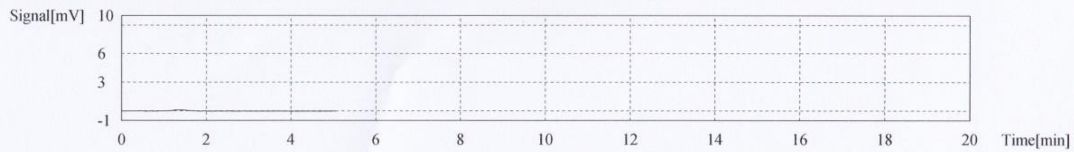
14/2/2015 2:17:05 PM

TOC-Control L Report

2015_02_14_001_hafiz.tlx

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	0.000	0.000	0.000ug	0.000%	181.1mg	181uL		240114_SSM_IC Std.2014_01_24_11_21_07.cal	14/2/2015 11:17:12 AM

Mean Area 0.000
Mean CNV 0.000
Mean Conc. 0.000%



Sample

Sample Name:	S3-1c
Sample ID:	Untitled
Origin:	240114_SSM TOC method.met
Status	Completed
Chk. Result	

Type	Anal.	Manual Dilution	Density	Result
Unknown	SSM-TOC	1.000	1.000mg/uL	SSM-TOC:-0.00724% SSM-TC:0.000% SSM-IC:0.00724%

1. Det

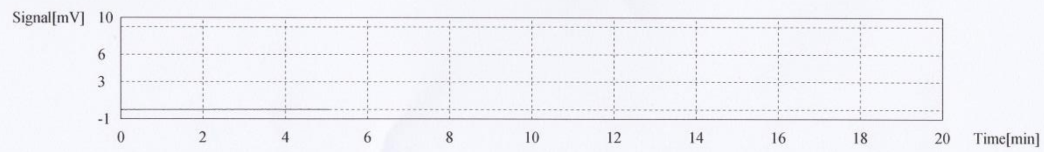
Anal.: SSM-TC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	0.000	0.000	0.000ug	0.000%	169.4mg	169uL		240114_SSM_TC Std.2014_01_24_10_16_26.cal	14/2/2015 11:26:55 AM

TOC-Control L Report

2015_02_14_001_hafiz.tlx

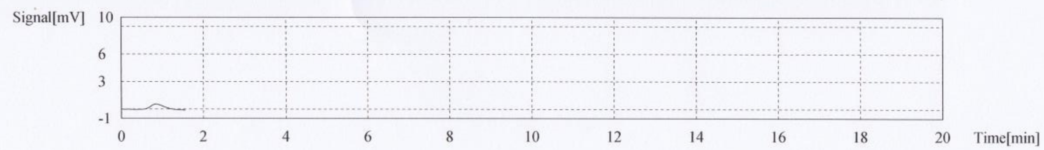
Mean Area 0.000
Mean CNV 0.000
Mean Conc. 0.000%



Anal.: SSM-IC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	1.338	1.338	11.71ug	0.00724%	161.7mg	161uL		240114_SSM_IC Std 2014_01_24_11_21_07.cal	14/2/2015 11:30:46 AM

Mean Area 1.338
Mean CNV 1.338
Mean Conc. 0.00724%



Sample

Sample Name: S1-1a
Sample ID: Untitled
Origin: 240114_SSM TOC method.met
Status Completed
Chk. Result

Type	Anal.	Manual Dilution	Density	Result
Unknown	SSM-TOC	1.000	1.000mg/uL	SSM-TOC:0.5455% SSM-TC:0.5595% SSM-IC:0.01400%

1. Det

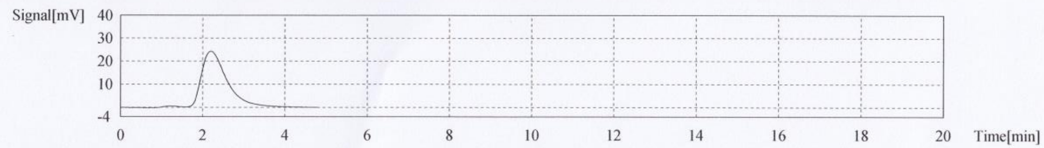
Anal.: SSM-TC

TOC-Control L Report

2015_02_14_001_hafiz.tlx

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	109.6	109.6	929.9ug	0.5595%	166.2mg	166uL		240114_SSM_TC Std.2014_01_24_10_16_26.cal	14/2/2015 12:07:10 PM

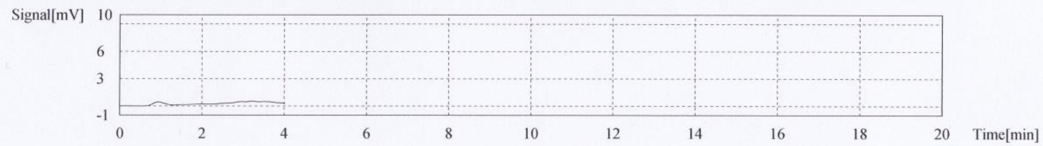
Mean Area 109.6
Mean CNV 109.6
Mean Conc. 0.5595%



Anal.: SSM-IC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	2.877	2.877	25.17ug	0.01400%	179.8mg	179uL		240114_SSM_IC Std.2014_01_24_11_21_07.cal	14/2/2015 12:21:27 PM

Mean Area 2.877
Mean CNV 2.877
Mean Conc. 0.01400%



Sample

Sample Name: S1-1b
Sample ID: Untitled
Origin: 240114_SSM TOC method.met
Status Completed
Chk. Result

Type	Anal.	Manual Dilution	Density	Result
Unknown	SSM-TOC	1.000	1.000mg/uL	SSM-TOC:0.00170% SSM-TC:0.00764% SSM-IC:0.00594%

5/16 14/2/2015 2:17:05 PM

TOC-Control L Report

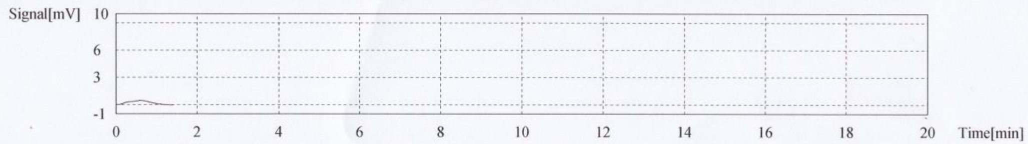
2015_02_14_001_hafiz.tlx

1. Det

Anal.: SSM-TC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	1.681	1.681	14.26ug	0.00764%	186.7mg	186uL		240114_SSM_TC Std.2014_01_24_10_16_26.cal	14/2/2015 12:25:50 PM

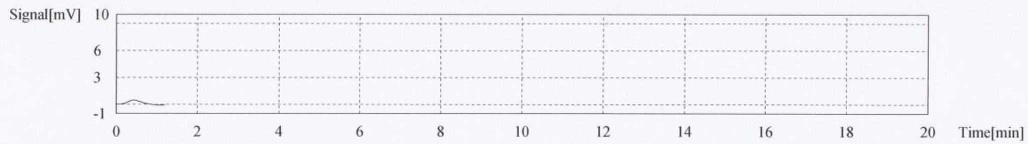
Mean Area 1.681
Mean CNV 1.681
Mean Conc. 0.00764%



Anal.: SSM-IC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	1.108	1.108	9.695ug	0.00594%	163.2mg	163uL		240114_SSM_IC Std.2014_01_24_11_21_07.cal	14/2/2015 12:29:18 PM

Mean Area 1.108
Mean CNV 1.108
Mean Conc. 0.00594%



Sample

Sample Name: S1-1c
Sample ID: Untitled
Origin: 240114_SSM TOC method.met
Status Completed
Chk. Result

TOC-Control L Report

2015_02_14_001_hafiz.tlx

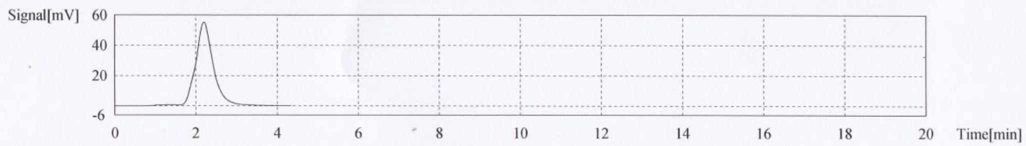
Type	Anal.	Manual Dilution	Density	Result
Unknown	SSM-TOC	1.000	1.000mg/uL	SSM-TOC:0.7954% SSM-TC:0.7994% SSM-IC:0.00404%

1. Det

Anal.: SSM-TC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	168.0	168.0	1425ug	0.7994%	178.3mg	178uL		240114_SSM_TC Std.2014_01_24_10_16_26.cal	14/2/2015 12:35:48 PM

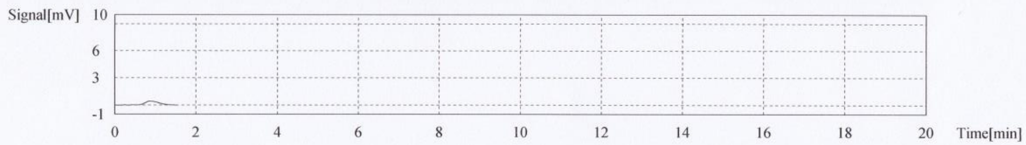
Mean Area 168.0
Mean CNV 168.0
Mean Conc. 0.7994%



Anal.: SSM-IC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	0.8891	0.8891	7.780ug	0.00404%	192.7mg	192uL		240114_SSM_IC Std.2014_01_24_11_21_07.cal	14/2/2015 12:39:05 PM

Mean Area 0.8891
Mean CNV 0.8891
Mean Conc. 0.00404%



Sample

TOC-Control L Report

2015_02_14_001_hafiz.tlx

Sample Name:	S2-1a
Sample ID:	Untitled
Origin:	240114_SSM TOC method.met
Status	Completed
Chk. Result	

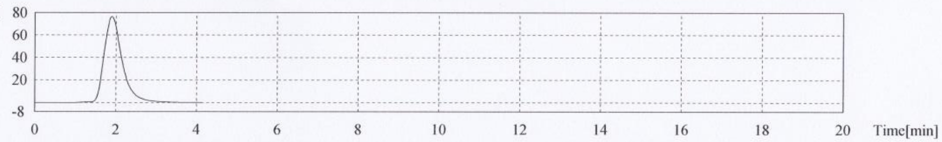
Type	Anal.	Manual Dilution	Density	Result
Unknown	SSM-TOC	1.000	1.000mg/uL	SSM-TOC:1.295% SSM-TC:1.303% SSM-IC:0.00782%

1. Det

Anal.: SSM-TC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	241.1	241.1	2046ug	1.303%	157.0mg	157uL		240114_SSM_TC Std.2014_01_24_10_16_26.cal	14/2/2015 12:45:39 PM

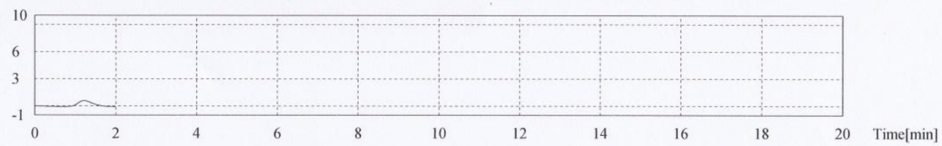
Mean Area 241.1
Mean CNV 241.1
Mean Conc. 1.303%



Anal.: SSM-IC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	1.534	1.534	13.42ug	0.00782%	171.6mg	171uL		240114_SSM_IC Std.2014_01_24_11_21_07.cal	14/2/2015 12:49:03 PM

Mean Area 1.534
Mean CNV 1.534
Mean Conc. 0.00782%



8/16

14/2/2015 2:17:05 PM

TOC-Control L Report

2015_02_14_001_hafiz.tlx

Sample

Sample Name:	S2-1b
Sample ID:	Untitled
Origin:	240114_SSM TOC method.met
Status	Completed
Chk. Result	

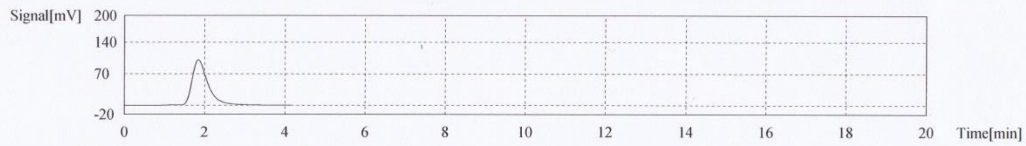
Type	Anal.	Manual Dilution	Density	Result
Unknown	SSM-TOC	1.000	1.000mg/uL	SSM-TOC:1.382% SSM-TC:1.389% SSM-IC:0.00713%

1. Det

Anal.: SSM-TC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	281.0	281.0	2384ug	1.389%	171.6mg	171uL		240114_SSM_TC Std.2014_01_24_10_16_26.cal	14/2/2015 12:55:14 PM

Mean Area	281.0
Mean CNV	281.0
Mean Conc.	1.389%



Anal.: SSM-IC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	1.249	1.249	10.93ug	0.00713%	153.3mg	153uL		240114_SSM_IC Std.2014_01_24_11_21_07.cal	14/2/2015 12:58:33 PM

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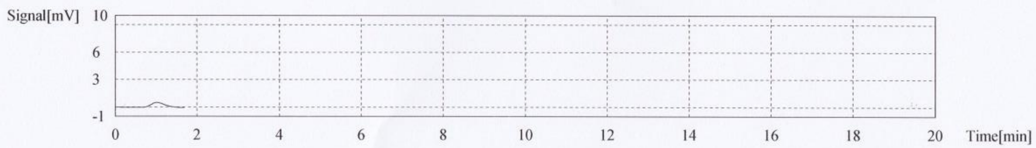
14/2/2015 2:17:05 PM

TOC-Control L Report

2015_02_14_001_hafiz.tlx

Mean Area 1.249
Mean CNV 1.249
Mean Conc. 0.00713%



Sample

Sample Name: S2-1c
Sample ID: Untitled
Origin: 240114_SSM TOC method.met
Status Completed
Chk. Result

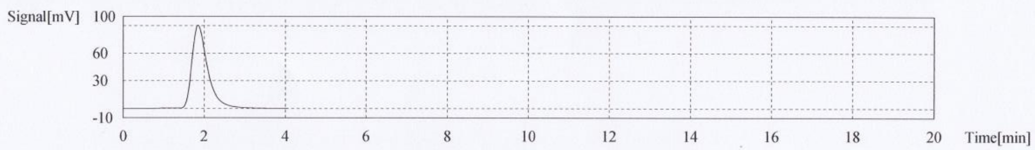
Type	Anal.	Manual Dilution	Density	Result
Unknown	SSM-TOC	1.000	1.000mg/uL	SSM-TOC:1.311% SSM-TC:1.317% SSM-IC:0.00610%

1. Det

Anal.: SSM-TC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	245.8	245.8	2085ug	1.317%	158.3mg	158uL		240114_SSM_TC Std.2014_01_24_10_16_26.cal	14/2/2015 1:04:30 PM

Mean Area 245.8
Mean CNV 245.8
Mean Conc. 1.317%



Anal.: SSM-IC

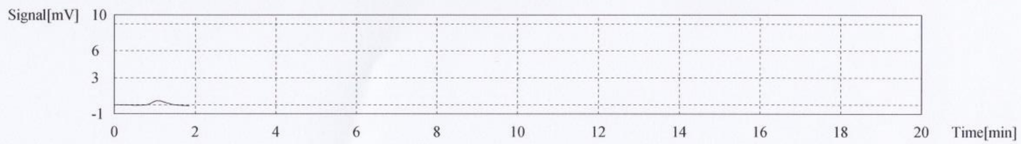
10/16 14/2/2015 2:17:05 PM

TOC-Control L Report

2015_02_14_001_hafiz.tlx

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	1.236	1.236	10.81ug	0.00610%	177.3mg	177uL		240114_SSM_IC Std.2014_01_24_11_21_07.cal	14/2/2015 1:08:04 PM

Mean Area 1.236
Mean CNV 1.236
Mean Conc. 0.00610%



Sample

Sample Name: S5-1a
Sample ID: Untitled
Origin: 240114_SSM TOC method.met
Status Completed
Chk. Result

Type	Anal.	Manual Dilution	Density	Result
Unknown	SSM-TOC	1.000	1.000mg/uL	SSM-TOC:0.3569% SSM-TC:0.3640% SSM-IC:0.00704%

1. Det

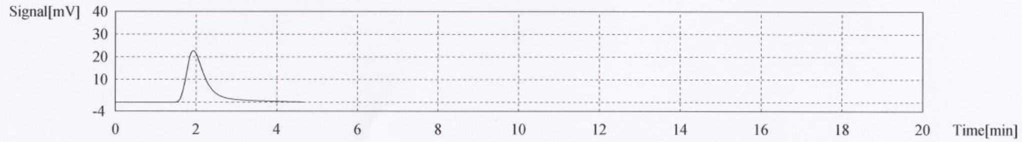
Anal.: SSM-TC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	78.29	78.29	664.2ug	0.3640%	182.5mg	182uL		240114_SSM_TC Std.2014_01_24_10_16_26.cal	14/2/2015 1:18:19 PM

TOC-Control L Report

2015_02_14_001_hafiz.tlx

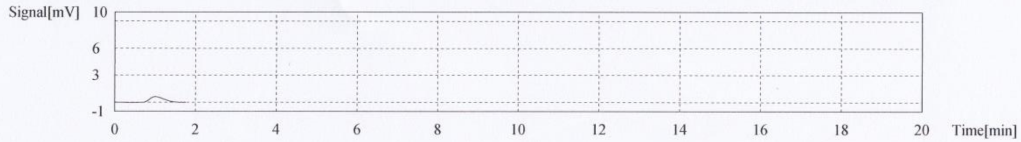
Mean Area	78.29
Mean CNV	78.29
Mean Conc.	0.3640%



Anal.: SSM-IC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	1.516	1.516	13.26ug	0.00704%	188.5mg	188uL		240114_SSM_IC Std.2014_01_24_11_21_07.cal	14/2/2015 1:22:40 PM

Mean Area	1.516
Mean CNV	1.516
Mean Conc.	0.00704%



Sample

Sample Name:	S5-1b
Sample ID:	Untitled
Origin:	240114_SSM TOC method.met
Status	Completed
Chk. Result	

Type	Anal.	Manual Dilution	Density	Result
Unknown	SSM-TOC	1.000	1.000mg/uL	SSM-TOC:0.1571% SSM-TC:0.1736% SSM-IC:0.01644%

1. Det

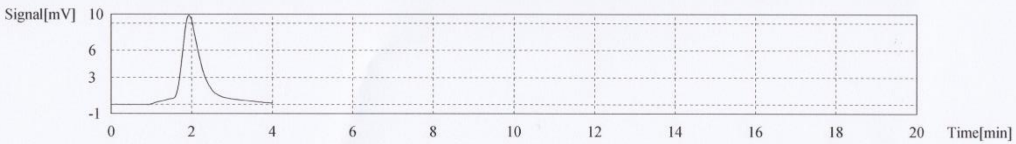
Anal.: SSM-TC

TOC-Control L Report

2015_02_14_001_hafiz.tlx

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	34.19	34.19	290.1ug	0.1736%	167.1mg	167uL		240114_SSM_TC Std.2014_01_24_10_16_26.cal	14/2/2015 1:30:36 PM

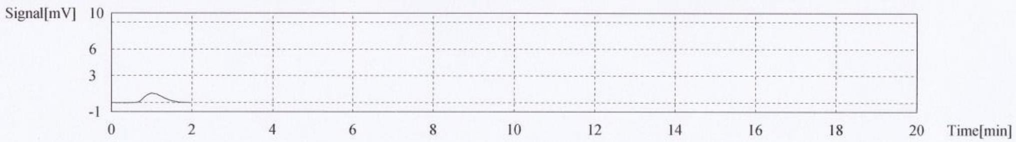
Mean Area 34.19
Mean CNV 34.19
Mean Conc. 0.1736%



Anal.: SSM-IC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	3.401	3.401	29.76ug	0.01644%	181.0mg	181uL		240114_SSM_IC Std.2014_01_24_11_21_07.cal	14/2/2015 1:34:40 PM

Mean Area 3.401
Mean CNV 3.401
Mean Conc. 0.01644%



Sample

Sample Name: S5-1c
Sample ID: Untitled
Origin: 240114_SSM TOC method.met
Status Completed
Chk. Result

Type	Anal.	Manual Dilution	Density	Result
Unknown	SSM-TOC	1.000	1.000mg/uL	SSM-TOC:0.2461% SSM-TC:0.2511% SSM-IC:0.00495%

TOC-Control L Report

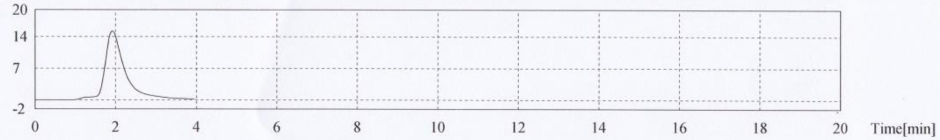
2015_02_14_001_hafiz.tlx

1. Det

Anal.: SSM-TC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	51.29	51.29	435.1ug	0.2511%	173.3mg	173uL		240114_SSM_TC Std.2014_01_24_10_16_26.cal	14/2/2015 1:40:41 PM

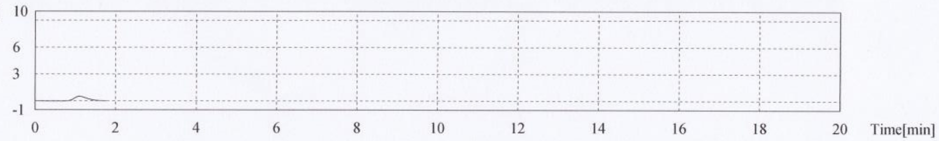
Mean Area 51.29
Mean CNV 51.29
Mean Conc. 0.2511%



Anal.: SSM-IC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	1.077	1.077	9.424ug	0.00495%	190.2mg	190uL		240114_SSM_IC Std.2014_01_24_11_21_07.cal	14/2/2015 1:43:50 PM

Mean Area 1.077
Mean CNV 1.077
Mean Conc. 0.00495%



Sample

Sample Name: S3-1b(correction)
Sample ID: Untitled
Origin: 240114_SSM TOC method.met
Status Completed
Chk. Result

TOC-Control L Report

2015_02_14_001_hafiz.tlx

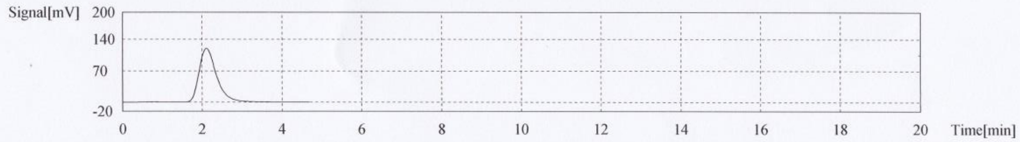
Type	Anal.	Manual Dilution	Density	Result
Unknown	SSM-TOC	1.000	1.000mg/uL	SSM-TOC:1.647% SSM-TC:1.653% SSM-IC:0.00632%

1. Det

Anal.: SSM-TC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	370.1	370.1	3140ug	1.653%	189.9mg	189uL		240114_SSM_TC Std.2014_01_24_10_16_26.cal	14/2/2015 1:53:56 PM

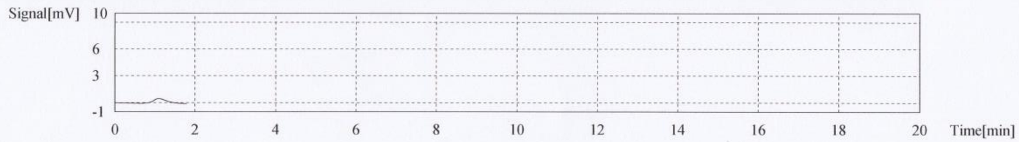
Mean Area 370.1
Mean CNV 370.1
Mean Conc. 1.653%



Anal.: SSM-IC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	1.115	1.115	9.756ug	0.00632%	154.4mg	154uL		240114_SSM_IC Std.2014_01_24_11_21_07.cal	14/2/2015 1:57:20 PM

Mean Area 1.115
Mean CNV 1.115
Mean Conc. 0.00632%



Sample

15/16

14/2/2015 2:17:05 PM

TOC-Control L Report

2015_02_14_001_hafiz.tlx

Sample Name:	S3-1c(correction)
Sample ID:	Untitled
Origin:	240114_SSM TOC method.met
Status	Completed
Chk. Result	

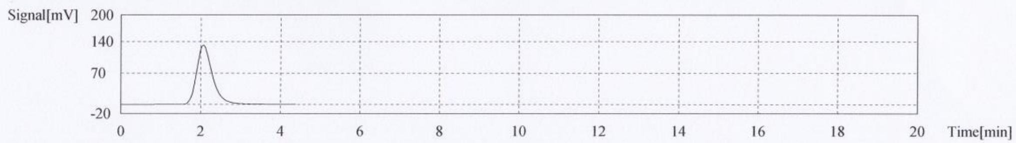
Type	Anal.	Manual Dilution	Density	Result
Unknown	SSM-TOC	1.000	1.000mg/uL	SSM-TOC:1.870% SSM-TC:1.870% SSM-IC:0.000%

1. Det

Anal.: SSM-TC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	367.9	367.9	3121ug	1.870%	166.9mg	166uL		240114_SSM_TC Std.2014_01_24_10_16_26.cal	14/2/2015 2:04:04 PM

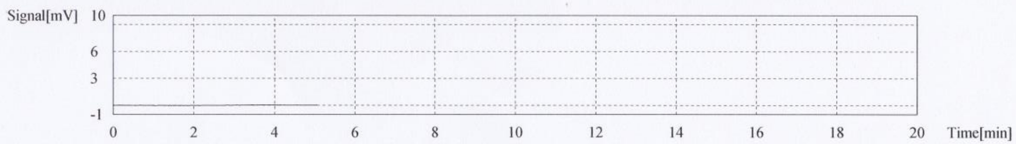
Mean Area 367.9
Mean CNV 367.9
Mean Conc. 1.870%



Anal.: SSM-IC

No.	Area	CNV	Abs C	Conc.	Weight	Volume	Ex.	Cal. Curve	Date / Time
1	0.000	0.000	0.000ug	0.000%	175.3mg	175uL		240114_SSM_IC Std.2014_01_24_11_21_07.cal	14/2/2015 2:12:41 PM

Mean Area 0.000
Mean CNV 0.000
Mean Conc. 0.000%



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APPENDIX 3

UV TEST RESULTS

Sample Vials	Absorption Rate		
	1st reading	2nd reading	3rd reading
1	0.080	0.079	0.079
2	0.143	0.142	0.142
3	0.113	0.113	0.113
4	0.071	0.070	0.071
5	0.108	0.108	0.108

APPENDIX 4

QWASI 3.10 INPUT AND FULL RESULTS

Benz(a)anthracene from Sampling Point S1 and S3

Benz(a)anthracene (Chemical Parameters) of Sampling Point S1

Chemical Type	1			
Molar Mass	228	g/mol		
Temperature	25.00	°C	298	K
Log Kow	5.91			
Solubility	9.00E-03	g/m³	3.94E-05	mol/m³
Vapour Pressure	3.73E-06	Pa		
Melting Point	161	°C	434	K
Sub-cooled Liquid				
Vapour Pressure	8.20E-05	Pa		
Fugacity Ratio	0.0455			
Henry's Law Constant	0.0946	Pa.m³/mol		

		L/kg
Air-Water (Kaw)	3.82E-05	-
Suspended Particles-Water	1.92E+05	79982
Sediment-Water	31993	13330
Resuspended Particles-Water	27994	11664
Aerosol-Air	7.32E+10	-
Organic Carbon-Water (Koc)	-	3.33E+05

	Half-Life	Rate Constant
	h	1/h
Water	4896	1.42E-04
Sediment	4776	1.45E-04

Benz(a)anthracene (Environmental Parameters) of Sampling Point S1

	Area	Depth	Volume
	m^2	m	m^3
Water	17100	3.00	51300
Sediment	17100	0.0400	684

	Inflow	Outflow
Water	900m^3/h	900m^3/h
Suspended Particles	0.0375m^3/h	0.0375m^3/h

Sediment Subcompartment Volumes, m^3

Solids	103
Pore-Water	581

	Density kg/m^3	Concentration of Particles	Volume Fraction	OC Fraction
Particles In Water Column	2400	100 mg/L	4.17E-05	0.24
Sediment Solids	2400		0.1500	0.04
Inflow Particles	2400	100 mg/L	4.17E-05	0.24
Resuspended Particles	2400			0.035
Aerosols In Air	1500	41.75 µg/m^3	2.78E-11	

Mass Transfer Coefficients	m/h
Volatilization (air side)	1.00
Volatilization (water side)	0.0100
Sediment-water Diffusion	4.00E-04
Aerosol Dry Deposition Velocity	7.20
Aerosol Scavenging Ratio	2.00E+05

	m^3/h	
Rain Rate	4.74	2.43 m/year
Sediment Deposition	5.09E-04	1.72 g/m^2day
Sediment Resuspension	1.78E-04	0.6000 g/m^2day
Sediment Burial	1.48E-04	0.5000 g/m^2day

Aerosol Deposition Rate	m^3/h
Wet	2.64E-05
Dry	3.43E-06
Total	2.98E-05

Benz(a)anthracene (Results) of Sampling Point S1

Emission	0	kg/year
Chemical Concentration in Inflow	2130	ng/L
Chemical Concentration in Air	0	ng/m³

Amounts

	mol	kg	%
Bulk Water	0.4689	0.1071	39.85
Water Solution	0.0521	0.0119	4.43
Water Particles	0.4168	0.0952	35.42
Bulk Sediment	0.7079	0.1616	60.15
Sediment Pore Water	1.25E-04	2.86E-05	0.0107
Sediment Solids	0.7078	0.1616	60.14
System Total	1.18	0.2687	4045

Amount Sorbed
(% of amount in bulk phase)

	%
Water	88.89
Sediment	99.98
Inflow	88.89
Air	67.07

	Fugacity	Z Values	Concentrations			
	Pa	mol/m³Pa	kg/m³			mol/(m³ of bulk)
Bulk Air	0	1.22E-03	0	0	ng/m³	
Air vapour		4.03E-04	0			
Aerosols		2.95E+07	0			0
Bulk Water	9.61E-08	95.11	2.09E-06	2087	ng/L	
Water Solution		10.57	2.32E-07			
Water Particles		2.03E+06	0.0445	18549	ng/g	8.13E-06
Bulk Inflow	9.81E-08	95.10	2.13E-06	2130	ng/L	
Inflow Water			2.37E-07			
Inflow Particles		2.03E+06	0.0454			8.29E-06
Bulk Sediment	2.04E-08	50731	2.36E-04	2.36E+08	ng/m³	
Sediment Pore Water			4.92E-08	49.22	ng/L	
Sediment Solids		3.38E+05	1.57E-03	656	ng/g	1.03E-03
Resuspended Solids		2.96E+05				
Rain	0		0	0	ng/L	

(•) kg/m³
( ) mol/m³

In the System

	mol/h	kg/year
Total Chemical Inputs	8.40E-03	16.79
Emission	0	0
Inflow	8.40E-03	16.79
Air to water transfer	0	0
Total Chemical Losses	8.40E-03	16.79
Outflow	8.23E-03	16.45
Water to air transfer	6.61E-07	1.32E-03
Total Transformation	1.69E-04	0.3381
Sediment Burial	1.02E-06	2.05E-03

(•) System
( ) Water
( ) Sediment

Residence Time (not including water-sediment exchange as a loss)

Water	56.54 h	2.36 d	6.45E-03 y
Sediment	6824 h	284 d	0.7790 y
System	140 h	5.84 d	0.0160 y

Emission to Water	0	Water to Sediment Diffusion	0.0139
Water Inflow	1.87	Sediment to Water Diffusion	2.95E-03
Particle Inflow	14.93		
		Water Transformation	0.1327
Rain Dissolution	0	Sediment Transformation	0.2054
Aerosol Deposition - Wet	0		
Aerosol Deposition - Dry	0	Sediment Burial	2.05E-03
Absorption	0	Water Outflow	1.83
Volatilization	1.32E-03	Particle Outflow	14.62
Sediment Deposition	0.1987		
Sediment Resuspension	2.15E-03		

(•) kg/year
( ) mol/h

	D Value mol/Pa.h	Response Time of Water years	Response Time of Sediment years
Burial	50.19		78.92
Sediment Transformation	5035		0.7867
Sediment Resuspension	52.70	10.57	75.16
Water To Sediment Diffusion	72.29	7.70	54.79
Sediment Deposition	1034	0.5389	3.83
Water Transformation	691	0.8065	
Volatilization	6.87	81.04	
Volat. (air side)	6.90		
Volat. (water side)	1807		
Water Outflow	9512	0.0585	
Water Particle Outflow	76083	7.32E-03	
Rain Dissolution	50.07	11.12	
Wet Particle Deposition	778	0.7155	
Dry Particle Deposition	101	5.51	
Water Inflow	9512	0.0585	
Water Particle Inflow	76083	7.32E-03	

(•) years
( ) days
( ) hours

Benz(a)anthracene (Chemical Parameters) Sampling Point S2

	Half-Life	Rate Constant
	h	1/h
Water	4896	1.42E-04
Sediment	4776	1.45E-04

		L/kg
Air-Water (Kaw)	3.82E-05	-
Suspended Particles-Water	1.92E+05	79982
Sediment-Water	31993	13330
Resuspended Particles-Water	27994	11664
Aerosol-Air	7.32E+10	-
Organic Carbon-Water (Koc)	-	3.33E+05

Chemical Type	1			
Molar Mass	228	g/mol		
Temperature	25.00	°C	298	K
Log Kow	5.91			
Solubility	9.00E-03	g/m³	3.94E-05	mol/m³
Vapour Pressure	3.73E-06	Pa		
Melting Point	161	°C	434	K
Sub-cooled Liquid				
Vapour Pressure	8.20E-05	Pa		
Fugacity Ratio	0.0455			
Henry's Law Constant	0.0946	Pa.m³/mol		

Benz(a)anthracene (Environmental Parameters) of Sampling Point S2

	Area	Depth	Volume
	m^2	m	m^3
Water	17100	3.00	51300
Sediment	17100	0.0400	684

	Inflow	Outflow
Water	900m³/h	900m³/h
Suspended Particles	0.0375m³/h	0.0375m³/h

Sediment Subcompartment Volumes, m³

Solids	103
Pore-Water	581

	Density kg/m³	Concentration of Particles	Volume Fraction	OC Fraction
Particles In Water Column	2400	100 mg/L	4.17E-05	0.24
Sediment Solids	2400		0.1500	0.04
Inflow Particles	2400	100 mg/L	4.17E-05	0.24
Resuspended Particles	2400			0.035
Aerosols In Air	1500	41.75 µg/m³	2.78E-11	

Mass Transfer Coefficients	m/h
Volatilization (air side)	1.00
Volatilization (water side)	0.0100
Sediment-water Diffusion	4.00E-04
Aerosol Dry Deposition Velocity	7.20
Aerosol Scavenging Ratio	2.00E+05

	m³/h	
Rain Rate	4.74	2.43 m/year
Sediment Deposition	5.09E-04	1.72 g/m²day
Sediment Resuspension	1.78E-04	0.6000 g/m²day
Sediment Burial	1.48E-04	0.5000 g/m²day

Aerosol Deposition Rate	m³/h
Wet	2.64E-05
Dry	3.43E-06
Total	2.98E-05

Benz(a)anthracene (Results) of Sampling Point S2

Amounts

	mol	kg	%
Bulk Water	0.1629	0.0372	39.85
Water Solution	0.0181	4.13E-03	4.43
Water Particles	0.1448	0.0331	35.42
Bulk Sediment	0.2459	0.0561	60.15
Sediment Pore Water	4.36E-05	9.94E-06	0.0107
Sediment Solids	0.2459	0.0561	60.14
System Total	0.4089	0.0933	4045

Amount Sorbed
(% of amount in bulk phase)

	%
Water	88.89
Sediment	99.98
Inflow	88.89
Air	67.07

Emission	0	kg/year
Chemical Concentration in Inflow	740	ng/L
Chemical Concentration in Air	0	ng/m³

	D Value mol/Pa.h	Response Time of Water years	Response Time of Sediment years
Burial	50.19		78.92
Sediment Transformation	5035		0.7867
Sediment Resuspension	52.70	10.57	75.16
Water To Sediment Diffusion	72.29	7.70	54.79
Sediment Deposition	1034	0.5389	3.83
Water Transformation	691	0.8065	
Volatilization	6.87	81.04	
Volat. (air side)	6.90		
Volat. (water side)	1807		
Water Outflow	9512	0.0585	
Water Particle Outflow	76083	7.32E-03	
Rain Dissolution	50.07	11.12	
Wet Particle Deposition	778	0.7155	
Dry Particle Deposition	101	5.51	
Water Inflow	9512	0.0585	
Water Particle Inflow	76083	7.32E-03	

(•) years
( ) days
( ) hours

	Fugacity	Z Values	Concentrations			
	Pa	mol/m³Pa	kg/m³			mol/(m³ of bulk)
Bulk Air	0	1.22E-03	0	0	ng/m³	
Air vapour		4.03E-04	0			
Aerosols		2.95E+07	0			0
Bulk Water	3.34E-08	95.11	7.25E-07	725	ng/L	
Water Solution		10.57	8.06E-08			
Water Particles		2.03E+06	0.0155	6444	ng/g	2.82E-06
Bulk Inflow	3.41E-08	95.10	7.40E-07	740	ng/L	
Inflow Water			8.22E-08			
Inflow Particles		2.03E+06	0.0158			2.88E-06
Bulk Sediment	7.09E-09	50731	8.21E-05	8.21E+07	ng/m³	
Sediment Pore Water			1.71E-08	17.10	ng/L	
Sediment Solids		3.38E+05	5.47E-04	228	ng/g	3.59E-04
Resuspended Solids		2.96E+05				
Rain	0		0	0	ng/L	

(•) kg/m³
( ) mol/m³

In the System

	mol/h	kg/year
Total Chemical Inputs	2.92E-03	5.83
Emission	0	0
Inflow	2.92E-03	5.83
Air to water transfer	0	0
Total Chemical Losses	2.92E-03	5.83
Outflow	2.86E-03	5.72
Water to air transfer	2.29E-07	4.59E-04
Total Transformation	5.87E-05	0.1175
Sediment Burial	3.56E-07	7.11E-04

(•) System
( ) Water
( ) Sediment

Residence Time (not including water-sediment exchange as a loss)

Water	56.54 h	2.36 d	6.45E-03 y
Sediment	6824 h	284 d	0.7790 y
System	140 h	5.84 d	0.0160 y

Emission to Water	0	Water to Sediment Diffusion	4.83E-03
Water Inflow	0.6484	Sediment to Water Diffusion	1.02E-03
Particle Inflow	5.19		
		Water Transformation	0.0461
Rain Dissolution	0	Sediment Transformation	0.0714
Aerosol Deposition - Wet	0		
Aerosol Deposition - Dry	0	Sediment Burial	7.11E-04
Absorption	0	Water Outflow	0.6352
Volatilization	4.59E-04	Particle Outflow	5.08
Sediment Deposition	0.0690		
Sediment Resuspension	7.47E-04		

(•) kg/year
( ) mol/h

APPENDIX 5

QWASI 3.10 INPUT AND FULL RESULTS

Benz(a)pyrene from S1,S2 and S3

Benzo(a)pyrene (Chemical Parameters) of Sampling Point S1

	Half-Life	Rate Constant
	h	1/h
Water	1700	4.08E-04
Sediment	55000	1.26E-05

		L/kg
Air-Water (Kaw)	1.87E-05	-
Suspended Particles-Water	2.59E+05	1.08E+05
Sediment-Water	43157	17982
Resuspended Particles-Water	37763	15734
Aerosol-Air	2.81E+11	-
Organic Carbon-Water (Koc)	-	4.50E+05

Chemical Type	1			
Molar Mass	252	g/mol		
Temperature	25.00	°C	298	K
Log Kow	6.04			
Solubility	3.80E-03	g/m³	1.51E-05	mol/m³
Vapour Pressure	7.00E-07	Pa		
Melting Point	175	°C	448	K
Sub-cooled Liquid				
Vapour Pressure	2.13E-05	Pa		
Fugacity Ratio	0.0328			
Henry's Law Constant	0.0465	Pa.m³/mol		

Benzo(a)pyrene (Environmental Parameters) of Sampling Point S1

	Area m^2	Depth m	Volume m^3
Water	17100	3.00	51300
Sediment	17100	0.0400	684

	Inflow	Outflow
Water	900m^3/h	900m^3/h
Suspended Particles	0.0375m^3/h	0.0375m^3/h

Sediment Subcompartment Volumes, m^3

Solids	103
Pore-Water	581

	Density kg/m^3	Concentration of Particles	Volume Fraction	OC Fraction
Particles In Water Column	2400	100 mg/L	4.17E-05	0.24
Sediment Solids	2400		0.1500	0.04
Inflow Particles	2400	100 mg/L	4.17E-05	0.24
Resuspended Particles	2400			0.035
Aerosols In Air	1500	41.75 µg/m^3	2.78E-11	

Mass Transfer Coefficients	m/h
Volatilization (air side)	1.00
Volatilization (water side)	0.0100
Sediment-water Diffusion	4.00E-04
Aerosol Dry Deposition Velocity	7.20
Aerosol Scavenging Ratio	2.00E+05

	m^3/h	
Rain Rate	4.74	2.43 m/year
Sediment Deposition	5.09E-04	1.72 g/m^2day
Sediment Resuspension	1.78E-04	0.6000 g/m^2day
Sediment Burial	1.48E-04	0.5000 g/m^2day

Aerosol Deposition Rate	m^3/h
Wet	2.64E-05
Dry	3.43E-06
Total	2.98E-05

Benzo(a)pyrene (Results) of Sampling Point S1

Amounts

	mol	kg	%
Bulk Water	2.90	0.7313	6.94
Water Solution	0.2459	0.0620	0.5887
Water Particles	2.65	0.6693	6.35
Bulk Sediment	38.87	9.81	93.06
Sediment Pore Water	5.10E-03	1.29E-03	0.0122
Sediment Solids	38.86	9.81	93.05
System Total	41.77	10.54	787

Amount Sorbed
(% of amount in bulk phase)

	%
Water	91.52
Sediment	99.99
Inflow	91.52
Air	88.68

Emission	0	kg/year
Chemical Concentration in Inflow	14740	ng/L
Chemical Concentration in Air	0	ng/m³

	D Value mol/Pa.h	Response Time of Water years	Response Time of Sediment years
Burial	138		78.91
Sediment Transformation	1201		9.06
Sediment Resuspension	145	10.26	75.16
Water To Sediment Diffusion	147	10.09	73.91
Sediment Deposition	2838	0.5234	3.83
Water Transformation	5305	0.2800	
Volatilization	6.89	216	
Volat. (air side)	6.90		
Volat. (water side)	3679		
Water Outflow	19365	0.0767	
Water Particle Outflow	2.09E+05	7.11E-03	
Rain Dissolution	102	14.57	
Wet Particle Deposition	2995	0.4960	
Dry Particle Deposition	389	3.82	
Water Inflow	19365	0.0767	
Water Particle Inflow	2.09E+05	7.11E-03	

(•) years
( ) days
( ) hours

	Fugacity	Z Values	Concentrations			
	Pa	mol/m³Pa	kg/m³			mol/(m³ of bulk)
Bulk Air	0	3.56E-03	0	0	ng/m³	
Air vapour		4.03E-04	0			
Aerosols		1.14E+08	0			0
Bulk Water	2.23E-07	254	1.43E-05	14256	ng/L	
Water Solution		21.52	1.21E-06			
Water Particles		5.57E+06	0.3131	1.30E+05	ng/g	5.17E-05
Bulk Inflow	2.30E-07	254	1.47E-05	14740	ng/L	
Inflow Water			1.25E-06			
Inflow Particles		5.57E+06	0.3238			5.35E-05
Bulk Sediment	4.08E-07	1.39E+05	0.0143	1.43E+10	ng/m³	
Sediment Pore Water			2.21E-06	2214	ng/L	
Sediment Solids		9.29E+05	0.0956	39819	ng/g	0.0568
Resuspended Solids		8.13E+05				
Rain	0		0	0	ng/L	

(•) kg/m³
( ) mol/m³

In the System

	mol/h	kg/year
Total Chemical Inputs	0.0526	116
Emission	0	0
Inflow	0.0526	116
Air to water transfer	0	0
Total Chemical Losses	0.0526	116
Outflow	0.0509	112
Water to air transfer	1.53E-06	3.39E-03
Total Transformation	1.67E-03	3.69
Sediment Burial	5.62E-05	0.1243

(•) System
( ) Water
( ) Sediment

Residence Time (not including water-sediment exchange as a loss)

Water	55.70 h	2.32 d	6.36E-03 y
Sediment	71192 h	2966 d	8.13 y
System	794 h	33.10 d	0.0907 y

Emission to Water	0	Water to Sediment Diffusion	0.0725
Water Inflow	9.86	Sediment to Water Diffusion	0.1327
Particle Inflow	106		
		Water Transformation	2.61
Rain Dissolution	0	Sediment Transformation	1.08
Aerosol Deposition - Wet	0		
Aerosol Deposition - Dry	0	Sediment Burial	0.1243
Absorption	0	Water Outflow	9.53
Volatilization	3.39E-03	Particle Outflow	103
Sediment Deposition	1.40		
Sediment Resuspension	0.1305		

(•) kg/year
( ) mol/h

Benzo(a)pyrene (Chemical Parameters) of Sampling Point S2

	Half-Life	Rate Constant
	h	1/h
Water	1700	4.08E-04
Sediment	55000	1.26E-05

		L/kg
Air-Water (Kaw)	1.87E-05	-
Suspended Particles-Water	2.59E+05	1.08E+05
Sediment-Water	43157	17982
Resuspended Particles-Water	37763	15734
Aerosol-Air	2.81E+11	-
Organic Carbon-Water (Koc)	-	4.50E+05

Chemical Type	1			
Molar Mass	252	g/mol		
Temperature	25.00	°C	298	K
Log Kow	6.04			
Solubility	3.80E-03	g/m³	1.51E-05	mol/m³
Vapour Pressure	7.00E-07	Pa		
Melting Point	175	°C	448	K
Sub-cooled Liquid				
Vapour Pressure	2.13E-05	Pa		
Fugacity Ratio	0.0328			
Henry's Law Constant	0.0465	Pa.m³/mol		

Benzo(a)pyrene (Environmental Parameters) of Sampling Point S2

	Area	Depth	Volume
	m^2	m	m^3
Water	17100	3.00	51300
Sediment	17100	0.0400	684

	Inflow	Outflow
Water	900m^3/h	900m^3/h
Suspended Particles	0.0375m^3/h	0.0375m^3/h

Sediment Subcompartment Volumes, m^3

Solids	103
Pore-Water	581

	Density kg/m^3	Concentration of Particles	Volume Fraction	OC Fraction
Particles In Water Column	2400	100 mg/L	4.17E-05	0.24
Sediment Solids	2400		0.1500	0.04
Inflow Particles	2400	100 mg/L	4.17E-05	0.24
Resuspended Particles	2400			0.035
Aerosols In Air	1500	41.75 µg/m^3	2.78E-11	

Mass Transfer Coefficients	m/h
Volatilization (air side)	1.00
Volatilization (water side)	0.0100
Sediment-water Diffusion	4.00E-04
Aerosol Dry Deposition Velocity	7.20
Aerosol Scavenging Ratio	2.00E+05

	m^3/h	
Rain Rate	4.74	2.43 m/year
Sediment Deposition	5.09E-04	1.72 g/m^2day
Sediment Resuspension	1.78E-04	0.6000 g/m^2day
Sediment Burial	1.48E-04	0.5000 g/m^2day

Aerosol Deposition Rate	m^3/h
Wet	2.64E-05
Dry	3.43E-06
Total	2.98E-05

Benzo(a)pyrene (Results) of Sampling Point S2

Amounts

	mol	kg	%
Bulk Water	0.7768	0.1960	6.94
Water Solution	0.0659	0.0166	0.5887
Water Particles	0.7109	0.1794	6.35
Bulk Sediment	10.42	2.63	93.06
Sediment Pore Water	1.37E-03	3.45E-04	0.0122
Sediment Solids	10.41	2.63	93.05
System Total	11.19	2.82	787

Amount Sorbed
(% of amount in bulk phase)

	%
Water	91.52
Sediment	99.99
Inflow	91.52
Air	88.68

Emission	0	kg/year
Chemical Concentration in Inflow	3950	ng/L
Chemical Concentration in Air	0	ng/m³

	D Value mol/Pa.h	Response Time of Water years	Response Time of Sediment years
Burial	138		78.91
Sediment Transformation	1201		9.06
Sediment Resuspension	145	10.26	75.16
Water To Sediment Diffusion	147	10.09	73.91
Sediment Deposition	2838	0.5234	3.83
Water Transformation	5305	0.2800	
Volatilization	6.89	216	
Volat. (air side)	6.90		
Volat. (water side)	3679		
Water Outflow	19365	0.0767	
Water Particle Outflow	2.09E+05	7.11E-03	
Rain Dissolution	102	14.57	
Wet Particle Deposition	2995	0.4960	
Dry Particle Deposition	389	3.82	
Water Inflow	19365	0.0767	
Water Particle Inflow	2.09E+05	7.11E-03	

(•) years
( ) days
( ) hours

	Fugacity Pa	Z Values mol/m³Pa	Concentrations kg/m³			mol/(m³ of bulk)
Bulk Air	0	3.56E-03	0	0	ng/m³	
Air vapour		4.03E-04	0			
Aerosols		1.14E+08	0			0
Bulk Water	5.97E-08	254	3.82E-06	3820	ng/L	
Water Solution		21.52	3.24E-07			
Water Particles		5.57E+06	0.0839	34962	ng/g	1.39E-05
Bulk Inflow	6.17E-08	254	3.95E-06	3950	ng/L	
Inflow Water			3.35E-07			
Inflow Particles		5.57E+06	0.0868			1.43E-05
Bulk Sediment	1.09E-07	1.39E+05	3.84E-03	3.84E+09	ng/m³	
Sediment Pore Water			5.93E-07	593	ng/L	
Sediment Solids		9.29E+05	0.0256	10671	ng/g	0.0152
Resuspended Solids		8.13E+05				
Rain	0		0	0	ng/L	

(•) kg/m³
( ) mol/m³

In the System

	mol/h	kg/year
Total Chemical Inputs	0.0141	31.14
Emission	0	0
Inflow	0.0141	31.14
Air to water transfer	0	0
Total Chemical Losses	0.0141	31.14
Outflow	0.0136	30.12
Water to air transfer	4.11E-07	9.08E-04
Total Transformation	4.48E-04	0.9899
Sediment Burial	1.51E-05	0.0333

(•) System
( ) Water
( ) Sediment

Residence Time (not including water-sediment exchange as a loss)

Water	55.70 h	2.32 d	6.36E-03 y
Sediment	71192 h	2966 d	8.13 y
System	794 h	33.10 d	0.0907 y

Emission to Water	0	Water to Sediment Diffusion	0.0194
Water Inflow	2.64	Sediment to Water Diffusion	0.0356
Particle Inflow	28.50		
		Water Transformation	0.6998
Rain Dissolution	0	Sediment Transformation	0.2901
Aerosol Deposition - Wet	0		
Aerosol Deposition - Dry	0	Sediment Burial	0.0333
Absorption	0	Water Outflow	2.55
Volatilization	9.08E-04	Particle Outflow	27.56
Sediment Deposition	0.3745		
Sediment Resuspension	0.0350		

(•) kg/year
( ) mol/h

Benzo(a)pyrene (Chemical Parameters) of Sampling Point S3

	Half-Life	Rate Constant
	h	1/h
Water	1700	4.08E-04
Sediment	55000	1.26E-05

		L/kg
Air-Water (Kaw)	1.87E-05	-
Suspended Particles-Water	2.59E+05	1.08E+05
Sediment-Water	43157	17982
Resuspended Particles-Water	37763	15734
Aerosol-Air	2.81E+11	-
Organic Carbon-Water (Koc)	-	4.50E+05

Chemical Type	1			
Molar Mass	252	g/mol		
Temperature	25.00	°C	298	K
Log Kow	6.04			
Solubility	3.80E-03	g/m^3	1.51E-05	mol/m^3
Vapour Pressure	7.00E-07	Pa		
Melting Point	175	°C	448	K
Sub-cooled Liquid Vapour Pressure	2.13E-05	Pa		
Fugacity Ratio	0.0328			
Henry's Law Constant	0.0465	$Pa.m^3/mol$		

Benzo(a)pyrene (Environmental Parameters) of Sampling Point S3

	Area	Depth	Volume
	m^2	m	m^3
Water	17100	3.00	51300
Sediment	17100	0.0400	684

	Inflow	Outflow
Water	$900 m^3/h$	$900 m^3/h$
Suspended Particles	$0.0375 m^3/h$	$0.0375 m^3/h$

Sediment Subcompartment Volumes, m^3

Solids	103
Pore-Water	581

	Density	Concentration	Volume	OC
	kg/m^3	of Particles	Fraction	Fraction
Particles In Water Column	2400	100 mg/L	4.17E-05	0.24
Sediment Solids	2400		0.1500	0.04
Inflow Particles	2400	100 mg/L	4.17E-05	0.24
Resuspended Particles	2400			0.035
Aerosols In Air	1500	$41.75\ \mu g/m^3$	2.78E-11	

Mass Transfer Coefficients	m/h
Volatilization (air side)	1.00
Volatilization (water side)	0.0100
Sediment-water Diffusion	4.00E-04
Aerosol Dry Deposition Velocity	7.20
Aerosol Scavenging Ratio	2.00E+05

	m^3/h	
Rain Rate	4.74	2.43 m/year
Sediment Deposition	5.09E-04	1.72 g/m^2day
Sediment Resuspension	1.78E-04	0.6000 g/m^2day
Sediment Burial	1.48E-04	0.5000 g/m^2day

Aerosol Deposition Rate	m^3/h
Wet	2.64E-05
Dry	3.43E-06
Total	2.98E-05

Benzo(a)pyrene (Results) of Sampling Point S3

Amounts

	mol	kg	%
Bulk Water	0.5251	0.1325	6.94
Water Solution	0.0445	0.0112	0.5887
Water Particles	0.4805	0.1212	6.35
Bulk Sediment	7.04	1.78	93.06
Sediment Pore Water	9.24E-04	2.33E-04	0.0122
Sediment Solids	7.04	1.78	93.05
System Total	7.57	1.91	787

Amount Sorbed
(% of amount in bulk phase)

	%
Water	91.52
Sediment	99.99
Inflow	91.52
Air	88.68

Emission	0	kg/year
Chemical Concentration in Inflow	2670	ng/L
Chemical Concentration in Air	0	ng/m³

	D Value mol/Pa.h	Response Time of Water years	Response Time of Sediment years
Burial	138		78.91
Sediment Transformation	1201		9.06
Sediment Resuspension	145	10.26	75.16
Water To Sediment Diffusion	147	10.09	73.91
Sediment Deposition	2838	0.5234	3.83
Water Transformation	5305	0.2800	
Volatilization	6.89	216	
Volat. (air side)	6.90		
Volat. (water side)	3679		
Water Outflow	19365	0.0767	
Water Particle Outflow	2.09E+05	7.11E-03	
Rain Dissolution	102	14.57	
Wet Particle Deposition	2995	0.4960	
Dry Particle Deposition	389	3.82	
Water Inflow	19365	0.0767	
Water Particle Inflow	2.09E+05	7.11E-03	

(•) years
( ) days
( ) hours

	Fugacity	Z Values	Concentrations			
	Pa	mol/m³Pa	kg/m³			mol/(m³ of bulk)
Bulk Air	0	3.56E-03	0	0	ng/m³	
Air vapour		4.03E-04	0			
Aerosols		1.14E+08	0			0
Bulk Water	4.03E-08	254	2.58E-06	2582	ng/L	
Water Solution		21.52	2.19E-07			
Water Particles		5.57E+06	0.0567	23633	ng/g	9.37E-06
Bulk Inflow	4.17E-08	254	2.67E-06	2670	ng/L	
Inflow Water			2.26E-07			
Inflow Particles		5.57E+06	0.0586			9.69E-06
Bulk Sediment	7.39E-08	1.39E+05	2.60E-03	2.60E+09	ng/m³	
Sediment Pore Water			4.01E-07	401	ng/L	
Sediment Solids		9.29E+05	0.0173	7213	ng/g	0.0103
Resuspended Solids		8.13E+05				
Rain	0		0	0	ng/L	

(•) kg/m³
( ) mol/m³

In the System

	mol/h	kg/year	
Total Chemical Inputs	9.52E-03	21.05	
Emission	0	0	
Inflow	9.52E-03	21.05	
Air to water transfer	0	0	
Total Chemical Losses	9.52E-03	21.05	
Outflow	9.21E-03	20.36	
Water to air transfer	2.78E-07	6.14E-04	
Total Transformation	3.03E-04	0.6691	
Sediment Burial	1.02E-05	0.0225	
Residence Time (not including water-sediment exchange as a loss)			
Water	55.70 h	2.32 d	6.36E-03 y
Sediment	71192 h	2966 d	8.13 y
System	794 h	33.10 d	0.0907 y

(•) System
( ) Water
( ) Sediment

Emission to Water	0	Water to Sediment Diffusion	0.0131
Water Inflow	1.79	Sediment to Water Diffusion	0.0240
Particle Inflow	19.27		
		Water Transformation	0.4731
Rain Dissolution	0	Sediment Transformation	0.1961
Aerosol Deposition - Wet	0		
Aerosol Deposition - Dry	0	Sediment Burial	0.0225
Absorption	0	Water Outflow	1.73
Volatilization	6.14E-04	Particle Outflow	18.63
Sediment Deposition	0.2531		
Sediment Resuspension	0.0236		

(•) kg/year
( ) mol/h

APPENDIX 6

QWASI 3.10 INPUT AND FULL RESULTS

Benzo(k)fluoranthene from S1, S2 and S3

Benzo(k)fluoranthene (Chemical Parameters) of Sampling Point S1

	Half-Life	Rate Constant
	h	1/h
Water	251	2.76E-03
Sediment	36600	1.89E-05

		L/kg
Air-Water (Kaw)	1.63E-06	-
Suspended Particles-Water	3.04E+05	1.27E+05
Sediment-Water	50706	21127
Resuspended Particles-Water	44367	18486
Aerosol-Air	6.09E+12	-
Organic Carbon-Water (Koc)	-	5.28E+05

Chemical Type	1			
Molar Mass	252	g/mol		
Temperature	25.00	°C	298	K
Log Kow	6.11			
Solubility	8.00E-04	g/m³	3.17E-06	mol/m³
Vapour Pressure	1.28E-08	Pa		
Melting Point	216	°C	489	K
Sub-cooled Liquid				
Vapour Pressure	9.85E-07	Pa		
Fugacity Ratio	0.0130			
Henry's Law Constant	4.04E-03	Pa.m³/mol		

Benzo(k)fluoranthene (Environmental Parameters) of Sampling Point S1

	Area m^2	Depth m	Volume m^3
Water	17100	3.00	51300
Sediment	17100	0.0400	684

	Inflow	Outflow
Water	900m^3/h	900m^3/h
Suspended Particles	0.0375m^3/h	0.0375m^3/h

Sediment Subcompartment Volumes, m^3

Solids	103
Pore-Water	581

	Density kg/m^3	Concentration of Particles	Volume Fraction	OC Fraction
Particles In Water Column	2400	100 mg/L	4.17E-05	0.24
Sediment Solids	2400		0.1500	0.04
Inflow Particles	2400	100 mg/L	4.17E-05	0.24
Resuspended Particles	2400			0.035
Aerosols In Air	1500	41.75 µg/m^3	2.78E-11	

Mass Transfer Coefficients	m/h
Volatilization (air side)	1.00
Volatilization (water side)	0.0100
Sediment-water Diffusion	4.00E-04
Aerosol Dry Deposition Velocity	7.20
Aerosol Scavenging Ratio	2.00E+05

	m^3/h	
Rain Rate	4.74	2.43 m/year
Sediment Deposition	5.09E-04	1.72 g/m^2day
Sediment Resuspension	1.78E-04	0.6000 g/m^2day
Sediment Burial	1.48E-04	0.5000 g/m^2day

Aerosol Deposition Rate	m^3/h
Wet	2.64E-05
Dry	3.43E-06
Total	2.98E-05

Benzo(k)fluoranthene (Results) of Sampling Point S1

Amounts

	mol	kg	%
Bulk Water	3.98	1.00	9.14
Water Solution	0.2911	0.0734	0.6686
Water Particles	3.69	0.9309	8.48
Bulk Sediment	39.55	9.98	90.86
Sediment Pore Water	4.42E-03	1.12E-03	0.0102
Sediment Solids	39.55	9.98	90.85
System Total	43.53	10.98	1005

Amount Sorbed
(% of amount in bulk phase)

	%
Water	92.69
Sediment	99.99
Inflow	92.69
Air	99.41

Emission	0	kg/year
Chemical Concentration in Inflow	22880	ng/L
Chemical Concentration in Air	0	ng/m³

	D Value mol/Pa.h	Response Time of Water years	Response Time of Sediment years
Burial	1864		78.91
Sediment Transformation	24403		6.03
Sediment Resuspension	1958	10.13	75.16
Water To Sediment Diffusion	1694	11.71	86.83
Sediment Deposition	38392	0.5168	3.83
Water Transformation	4.79E+05	0.0414	
Volatilization	6.90	2876	
Volat. (air side)	6.90		
Volat. (water side)	42359		
Water Outflow	2.23E+05	0.0890	
Water Particle Outflow	2.83E+06	7.02E-03	
Rain Dissolution	1174	16.91	
Wet Particle Deposition	64823	0.3061	
Dry Particle Deposition	8423	2.36	
Water Inflow	2.23E+05	0.0890	
Water Particle Inflow	2.83E+06	7.02E-03	

(•) years
( ) days
( ) hours

	Fugacity	Z Values	Concentrations			
	Pa	mol/m³Pa	kg/m³			mol/(m³ of bulk)
Bulk Air	0	0.0688	0	0	ng/m³	
Air vapour		4.03E-04	0			
Aerosols		2.46E+09	0			0
Bulk Water	2.29E-08	3388	1.96E-05	19579	ng/L	
Water Solution		248	1.43E-06			
Water Particles		7.54E+07	0.4355	1.81E+05	ng/g	7.19E-05
Bulk Inflow	2.68E-08	3388	2.29E-05	22880	ng/L	
Inflow Water			1.67E-06			
Inflow Particles		7.54E+07	0.5090			8.41E-05
Bulk Sediment	3.07E-08	1.88E+06	0.0146	1.46E+10	ng/m³	
Sediment Pore Water			1.92E-06	1918	ng/L	
Sediment Solids		1.26E+07	0.0973	40523	ng/g	0.0578
Resuspended Solids		1.10E+07				
Rain	0		0	0	ng/L	

(•) kg/m³
( ) mol/m³

In the System

	mol/h	kg/year
Total Chemical Inputs	0.0816	180
Emission	0	0
Inflow	0.0816	180
Air to water transfer	0	0
Total Chemical Losses	0.0816	180
Outflow	0.0698	154
Water to air transfer	1.58E-07	3.49E-04
Total Transformation	0.0117	25.91
Sediment Burial	5.72E-05	0.1265

(•) System
( ) Water
( ) Sediment

Residence Time (not including water-sediment exchange as a loss)

Water	49.26 h	2.05 d	5.62E-03 y
Sediment	49065 h	2044 d	5.60 y
System	533 h	22.22 d	0.0609 y

Emission to Water	0	Water to Sediment Diffusion	0.0858
Water Inflow	13.19	Sediment to Water Diffusion	0.1149
Particle Inflow	167		
		Water Transformation	24.25
Rain Dissolution	0	Sediment Transformation	1.66
Aerosol Deposition - Wet	0		
Aerosol Deposition - Dry	0	Sediment Burial	0.1265
Absorption	0	Water Outflow	11.29
Volatilization	3.49E-04	Particle Outflow	143
Sediment Deposition	1.94		
Sediment Resuspension	0.1328		

(•) kg/year
( ) mol/h

Benzo(k)fluoranthene (Chemical Parameters) of Sampling Point S2

	Half-Life	Rate Constant
	h	1/h
Water	251	2.76E-03
Sediment	36600	1.89E-05

		L/kg
Air-Water (Kaw)	1.63E-06	-
Suspended Particles-Water	3.04E+05	1.27E+05
Sediment-Water	50706	21127
Resuspended Particles-Water	44367	18486
Aerosol-Air	6.09E+12	-
Organic Carbon-Water (Koc)	-	5.28E+05

Chemical Type	1			
Molar Mass	252	g/mol		
Temperature	25.00	°C	298	K
Log Kow	6.11			
Solubility	8.00E-04	g/m^3	3.17E-06	mol/m^3
Vapour Pressure	1.28E-08	Pa		
Melting Point	216	°C	489	K
Sub-cooled Liquid				
Vapour Pressure	9.85E-07	Pa		
Fugacity Ratio	0.0130			
Henry's Law Constant	4.04E-03	$Pa.m^3/mol$		

Benzo(k)fluoranthene (Environmental Parameters) of Sampling Point S2

	Area	Depth	Volume
	m²	m	m³
Water	17100	3.00	51300
Sediment	17100	0.0400	684

	Inflow	Outflow
Water	900m³/h	900m³/h
Suspended Particles	0.0375m³/h	0.0375m³/h

Sediment Subcompartment Volumes, m³

Solids	103
Pore-Water	581

	Density kg/m³	Concentration of Particles	Volume Fraction	OC Fraction
Particles In Water Column	2400	100 mg/L	4.17E-05	0.24
Sediment Solids	2400		0.1500	0.04
Inflow Particles	2400	100 mg/L	4.17E-05	0.24
Resuspended Particles	2400			0.035
Aerosols In Air	1500	41.75 µg/m³	2.78E-11	

Mass Transfer Coefficients	m/h
Volatilization (air side)	1.00
Volatilization (water side)	0.0100
Sediment-water Diffusion	4.00E-04
Aerosol Dry Deposition Velocity	7.20
Aerosol Scavenging Ratio	2.00E+05

	m³/h	
Rain Rate	4.74	2.43 m/year
Sediment Deposition	5.09E-04	1.72 g/m²day
Sediment Resuspension	1.78E-04	0.6000 g/m²day
Sediment Burial	1.48E-04	0.5000 g/m²day

Aerosol Deposition Rate	m³/h
Wet	2.64E-05
Dry	3.43E-06
Total	2.98E-05

Benzo(k)fluoranthene (Results) of Sampling Point S2

Amounts

	mol	kg	%
Bulk Water	0.7429	0.1874	9.14
Water Solution	0.0543	0.0137	0.6686
Water Particles	0.6886	0.1737	8.48
Bulk Sediment	7.38	1.86	90.86
Sediment Pore Water	8.25E-04	2.08E-04	0.0102
Sediment Solids	7.38	1.86	90.85
System Total	8.12	2.05	1005

Amount Sorbed
(% of amount in bulk phase)

	%
Water	92.69
Sediment	99.99
Inflow	92.69
Air	99.41

Emission	0	kg/year
Chemical Concentration in Inflow	4270	ng/L
Chemical Concentration in Air	0	ng/m³

	D Value mol/Pa.h	Response Time of Water years	Response Time of Sediment years
Burial	1864		78.91
Sediment Transformation	24403		6.03
Sediment Resuspension	1958	10.13	75.16
Water To Sediment Diffusion	1694	11.71	86.83
Sediment Deposition	38392	0.5168	3.83
Water Transformation	4.79E+05	0.0414	
Volatilization	6.90	2876	
Volat. (air side)	6.90		
Volat. (water side)	42359		
Water Outflow	2.23E+05	0.0890	
Water Particle Outflow	2.83E+06	7.02E-03	
Rain Dissolution	1174	16.91	
Wet Particle Deposition	64823	0.3061	
Dry Particle Deposition	8423	2.36	
Water Inflow	2.23E+05	0.0890	
Water Particle Inflow	2.83E+06	7.02E-03	

years
days
hours

	Fugacity	Z Values	Concentrations			
	Pa	mol/m³Pa	kg/m³			mol/(m³ of bulk)
Bulk Air	0	0.0688	0	0	ng/m³	
Air vapour		4.03E-04	0			
Aerosols		2.46E+09	0			0
Bulk Water	4.27E-09	3388	3.65E-06	3654	ng/L	
Water Solution		248	2.67E-07			
Water Particles		7.54E+07	0.0813	33867	ng/g	1.34E-05
Bulk Inflow	5.00E-09	3388	4.27E-06	4270	ng/L	
Inflow Water			3.12E-07			
Inflow Particles		7.54E+07	0.0950			1.57E-05
Bulk Sediment	5.73E-09	1.88E+06	2.72E-03	2.72E+09	ng/m³	
Sediment Pore Water			3.58E-07	358	ng/L	
Sediment Solids		1.26E+07	0.0182	7563	ng/g	0.0108
Resuspended Solids		1.10E+07				
Rain	0		0	0	ng/L	

(•) kg/m³
( ) mol/m³

In the System

	mol/h	kg/year
Total Chemical Inputs	0.0152	33.67
Emission	0	0
Inflow	0.0152	33.67
Air to water transfer	0	0
Total Chemical Losses	0.0152	33.67
Outflow	0.0130	28.81
Water to air transfer	2.95E-08	6.52E-05
Total Transformation	2.19E-03	4.84
Sediment Burial	1.07E-05	0.0236

(•) System
( ) Water
( ) Sediment

Residence Time (not including water-sediment exchange as a loss)

Water	49.26 h	2.05 d	5.62E-03 y
Sediment	49065 h	2044 d	5.60 y
System	533 h	22.22 d	0.0609 y

Emission to Water	0	Water to Sediment Diffusion	0.0160
Water Inflow	2.46	Sediment to Water Diffusion	0.0214
Particle Inflow	31.20		
		Water Transformation	4.53
Rain Dissolution	0	Sediment Transformation	0.3089
Aerosol Deposition - Wet	0		
Aerosol Deposition - Dry	0	Sediment Burial	0.0236
Absorption	0	Water Outflow	2.11
Volatilization	6.52E-05	Particle Outflow	26.70
Sediment Deposition	0.3627		
Sediment Resuspension	0.0248		

(•) kg/year
( ) mol/h

Benzo(k)fluoranthene (Chemical Parameters) of Sampling Point S3

	Half-Life	Rate Constant
	h	1/h
Water	251	2.76E-03
Sediment	36600	1.89E-05

		L/kg
Air-Water (Kaw)	1.63E-06	-
Suspended Particles-Water	3.04E+05	1.27E+05
Sediment-Water	50706	21127
Resuspended Particles-Water	44367	18486
Aerosol-Air	6.09E+12	-
Organic Carbon-Water (Koc)	-	5.28E+05

Chemical Type	1			
Molar Mass	252	g/mol		
Temperature	25.00	°C	298	K
Log Kow	6.11			
Solubility	8.00E-04	g/m^3	3.17E-06	mol/m^3
Vapour Pressure	1.28E-08	Pa		
Melting Point	216	°C	489	K
Sub-cooled Liquid				
Vapour Pressure	9.85E-07	Pa		
Fugacity Ratio	0.0130			
Henry's Law Constant	4.04E-03	$Pa.m^3/mol$		

Benzo(k)fluoranthene (Environmental Parameters) Sampling Point S3

	Area	Depth	Volume
	m^2	m	m^3
Water	17100	3.00	51300
Sediment	17100	0.0400	684

	Inflow	Outflow
Water	$900 m^3/h$	$900 m^3/h$
Suspended Particles	$0.0375 m^3/h$	$0.0375 m^3/h$

Sediment Subcompartment Volumes, m^3

Solids	103
Pore-Water	581

	Density kg/m^3	Concentration of Particles	Volume Fraction	OC Fraction
Particles In Water Column	2400	100 mg/L	4.17E-05	0.24
Sediment Solids	2400		0.1500	0.04
Inflow Particles	2400	100 mg/L	4.17E-05	0.24
Resuspended Particles	2400			0.035
Aerosols In Air	1500	$41.75\ \mu g/m^3$	2.78E-11	

Mass Transfer Coefficients	m/h
Volatilization (air side)	1.00
Volatilization (water side)	0.0100
Sediment-water Diffusion	4.00E-04
Aerosol Dry Deposition Velocity	7.20
Aerosol Scavenging Ratio	2.00E+05

	m^3/h	
Rain Rate	4.74	2.43 m/year
Sediment Deposition	5.09E-04	1.72 g/m^2day
Sediment Resuspension	1.78E-04	0.6000 g/m^2day
Sediment Burial	1.48E-04	0.5000 g/m^2day

Aerosol Deposition Rate	m^3/h
Wet	2.64E-05
Dry	3.43E-06
Total	2.98E-05

Benzo(k)fluoranthene (Results) of Sampling Point S3

Amounts

	mol	kg	%
Bulk Water	2.40	0.6045	9.14
Water Solution	0.1752	0.0442	0.6686
Water Particles	2.22	0.5603	8.48
Bulk Sediment	23.80	6.01	90.86
Sediment Pore Water	2.66E-03	6.71E-04	0.0102
Sediment Solids	23.80	6.01	90.85
System Total	26.20	6.61	1005

Amount Sorbed (% of amount in bulk phase)

	%
Water	92.69
Sediment	99.99
Inflow	92.69
Air	99.41

Emission	0	kg/year
Chemical Concentration in Inflow	13770	ng/L
Chemical Concentration in Air	0	ng/m³

	D Value mol/Pa.h	Response Time of Water years	Response Time of Sediment years
Burial	1864		78.91
Sediment Transformation	24403		6.03
Sediment Resuspension	1958	10.13	75.16
Water To Sediment Diffusion	1694	11.71	86.83
Sediment Deposition	38392	0.5168	3.83
Water Transformation	4.79E+05	0.0414	
Volatilization	6.90	2876	
Volat. (air side)	6.90		
Volat. (water side)	42359		
Water Outflow	2.23E+05	0.0890	
Water Particle Outflow	2.83E+06	7.02E-03	
Rain Dissolution	1174	16.91	
Wet Particle Deposition	64823	0.3061	
Dry Particle Deposition	8423	2.36	
Water Inflow	2.23E+05	0.0890	
Water Particle Inflow	2.83E+06	7.02E-03	

- (•) years
- ( ) days
- ( ) hours

	Fugacity	Z Values	Concentrations			
	Pa	mol/m³Pa	kg/m³			mol/(m³ of bulk)
Bulk Air	0	0.0688	0	0	ng/m³	
Air vapour		4.03E-04	0			
Aerosols		2.46E+09	0			0
Bulk Water	1.38E-08	3388	1.18E-05	11783	ng/L	
Water Solution		248	8.62E-07			
Water Particles		7.54E+07	0.2621	1.09E+05	ng/g	4.33E-05
Bulk Inflow	1.61E-08	3388	1.38E-05	13770	ng/L	
Inflow Water			1.01E-06			
Inflow Particles		7.54E+07	0.3063			5.06E-05
Bulk Sediment	1.85E-08	1.88E+06	8.78E-03	8.78E+09	ng/m³	
Sediment Pore Water			1.15E-06	1154	ng/L	
Sediment Solids		1.26E+07	0.0585	24388	ng/g	0.0348
Resuspended Solids		1.10E+07				
Rain	0		0	0	ng/L	

(•) kg/m³
( ) mol/m³

In the System

	mol/h	kg/year
Total Chemical Inputs	0.0491	109
Emission	0	0
Inflow	0.0491	109
Air to water transfer	0	0
Total Chemical Losses	0.0491	109
Outflow	0.0420	92.90
Water to air transfer	9.51E-08	2.10E-04
Total Transformation	7.05E-03	15.59
Sediment Burial	3.44E-05	0.0761

(•) System
( ) Water
( ) Sediment

Residence Time (not including water-sediment exchange as a loss)

Water	49.26 h	2.05 d	5.62E-03 y
Sediment	49065 h	2044 d	5.60 y
System	533 h	22.22 d	0.0609 y

Emission to Water	0	Water to Sediment Diffusion	0.0516
Water Inflow	7.94	Sediment to Water Diffusion	0.0692
Particle Inflow	101		
		Water Transformation	14.60
Rain Dissolution	0	Sediment Transformation	0.9962
Aerosol Deposition - Wet	0		
Aerosol Deposition - Dry	0	Sediment Burial	0.0761
Absorption	0	Water Outflow	6.79
Volatilization	2.10E-04	Particle Outflow	86.11
Sediment Deposition	1.17		
Sediment Resuspension	0.0799		

(•) kg/year
( ) mol/h

APPENDIX 7

QWASI 3.10 INPUT AND FULL RESULTS

Chrysene from S1 and S3

Chrysene (Chemical Parameters) of Sampling Point S1

	Half-Life	Rate Constant
	h	1/h
Water	9.00	0.0770
Sediment	8760	7.91E-05

		L/kg
Air-Water (Kaw)	4.32E-03	-
Suspended Particles-Water	1.46E+05	60673
Sediment-Water	24269	10112
Resuspended Particles-Water	21236	8848
Aerosol-Air	3.88E+08	-
Organic Carbon-Water (Koc)	-	2.53E+05

Chemical Type	1			
Molar Mass	228	g/mol		
Temperature	25.00	°C	298	K
Log Kow	5.79			
Solubility	1.79E-03	g/m³	7.84E-06	mol/m³
Vapour Pressure	8.40E-05	Pa		
Melting Point	254	°C	527	K
Sub-cooled Liquid				
Vapour Pressure	0.0155	Pa		
Fugacity Ratio	5.43E-03			
Henry's Law Constant	10.71	Pa.m³/mol		

Chrysene (Environmental Parameters) Sampling Point S1

	Area	Depth	Volume
	m^2	m	m^3
Water	17100	3.00	51300
Sediment	17100	0.0400	684

	Inflow	Outflow
Water	900m^3/h	900m^3/h
Suspended Particles	0.0375m^3/h	0.0375m^3/h

Sediment Subcompartment Volumes, m^3

Solids	103
Pore-Water	581

	Density	Concentration	Volume	OC
	kg/m^3	of Particles	Fraction	Fraction
Particles In Water Column	2400	100 mg/L	4.17E-05	0.24
Sediment Solids	2400		0.1500	0.04
Inflow Particles	2400	100 mg/L	4.17E-05	0.24
Resuspended Particles	2400			0.035
Aerosols In Air	1500	41.75 µg/m^3	2.78E-11	

Mass Transfer Coefficients	m/h
Volatilization (air side)	1.00
Volatilization (water side)	0.0100
Sediment-water Diffusion	4.00E-04
Aerosol Dry Deposition Velocity	7.20
Aerosol Scavenging Ratio	2.00E+05

	m^3/h	
Rain Rate	4.74	2.43 m/year
Sediment Deposition	5.09E-04	1.72 g/m^2day
Sediment Resuspension	1.78E-04	0.6000 g/m^2day
Sediment Burial	1.48E-04	0.5000 g/m^2day

Aerosol Deposition Rate	m^3/h
Wet	2.64E-05
Dry	3.43E-06
Total	2.98E-05

Chrysene (Results) of Sampling Point S1

Emission	0	kg/year
Chemical Concentration in Inflow	2880	ng/L
Chemical Concentration in Air	0	ng/m³

	D Value mol/Pa.h	Response Time of Water years	Response Time of Sediment years
Burial	0.3363		78.92
Sediment Transformation	18.39		1.44
Sediment Resuspension	0.3531	10.94	75.16
Water To Sediment Diffusion	0.6385	6.05	41.57
Sediment Deposition	6.92	0.5579	3.83
Water Transformation	2606	1.48E-03	
Volatilization	4.82	0.8020	
Volat. (air side)	6.90		
Volat. (water side)	15.96		
Water Outflow	84.01	0.0460	
Water Particle Outflow	510	7.58E-03	
Rain Dissolution	0.4422	8.74	
Wet Particle Deposition	4.13	0.9356	
Dry Particle Deposition	0.5365	7.20	
Water Inflow	84.01	0.0460	
Water Particle Inflow	510	7.58E-03	

(•) years
( ) days
( ) hours

In the System

	mol/h	kg/year
Total Chemical Inputs	0.0114	22.71
Emission	0	0
Inflow	0.0114	22.71
Air to water transfer	0	0
Total Chemical Losses	0.0114	22.71
Outflow	2.10E-03	4.20
Water to air transfer	1.70E-05	0.0341
Total Transformation	9.24E-03	18.47
Sediment Burial	4.56E-07	9.12E-04

(•) System
( ) Water
( ) Sediment

Residence Time (not including water-sediment exchange as a loss)

Water	10.56 h	0.4400 d	1.21E-03 y
Sediment	12414 h	517 d	1.42 y
System	38.30 h	1.60 d	4.37E-03 y

Emission to Water	0	Water to Sediment Diffusion	4.51E-03
Water Inflow	3.21	Sediment to Water Diffusion	1.73E-03
Particle Inflow	19.49		
		Water Transformation	18.42
Rain Dissolution	0	Sediment Transformation	0.0499
Aerosol Deposition - Wet	0		
Aerosol Deposition - Dry	0	Sediment Burial	9.12E-04
Absorption	0	Water Outflow	0.5940
Volatilization	0.0341	Particle Outflow	3.60
Sediment Deposition	0.0490		
Sediment Resuspension	9.57E-04		

kg/year
mol/h

Amounts

	mol	kg	%
Bulk Water	0.1196	0.0273	27.51
Water Solution	0.0169	3.86E-03	3.89
Water Particles	0.1027	0.0234	23.62
Bulk Sediment	0.3152	0.0720	72.49
Sediment Pore Water	7.36E-05	1.68E-05	0.0169
Sediment Solids	0.3152	0.0719	72.47
System Total	0.4349	0.0993	2824

Amount Sorbed
(% of amount in bulk phase)

	%
Water	85.85
Sediment	99.98
Inflow	85.85
Air	1.07

	Fugacity Pa	Z Values mol/m³Pa	Concentrations kg/m³			mol/(m³ of bulk)
Bulk Air	0	4.08E-04	0	0	ng/m³	
Air vapour		4.03E-04	0			
Aerosols		1.57E+05	0			0
Bulk Water	3.54E-06	0.6597	5.32E-07	532	ng/L	
Water Solution		0.0933	7.53E-08			
Water Particles		13592	0.0110	4571	ng/g	2.00E-06
Bulk Inflow	1.91E-05	0.6597	2.88E-06	2880	ng/L	
Inflow Water			4.08E-07			
Inflow Particles		13592	0.0593			1.08E-05
Bulk Sediment	1.36E-06	340	1.05E-04	1.05E+08	ng/m³	
Sediment Pore Water			2.89E-08	28.89	ng/L	
Sediment Solids		2265	7.01E-04	292	ng/g	4.61E-04
Resuspended Solids		1982				
Rain	0		0	0	ng/L	

kg/m³
mol/m³

Chrysene (Chemical Parameters) of Sampling Point S3

	Half-Life	Rate Constant
	h	1/h
Water	9.00	0.0770
Sediment	8760	7.91E-05

		L/kg
Air-Water (Kaw)	4.32E-03	-
Suspended Particles-Water	1.46E+05	60673
Sediment-Water	24269	10112
Resuspended Particles-Water	21236	8848
Aerosol-Air	3.88E+08	-
Organic Carbon-Water (Koc)	-	2.53E+05

Chemical Type	1			
Molar Mass	228	g/mol		
Temperature	25.00	°C	298	K
Log Kow	5.79			
Solubility	1.79E-03	g/m^3	7.84E-06	mol/m^3
Vapour Pressure	8.40E-05	Pa		
Melting Point	254	°C	527	K
Sub-cooled Liquid				
Vapour Pressure	0.0155	Pa		
Fugacity Ratio	5.43E-03			
Henry's Law Constant	10.71	$Pa.m^3/mol$		

Chrysene (Environmental Parameters) of Sampling Point S3

	Area m^2	Depth m	Volume m^3
Water	17100	3.00	51300
Sediment	17100	0.0400	684

	Inflow	Outflow
Water	900m^3/h	900m^3/h
Suspended Particles	0.0375m^3/h	0.0375m^3/h

Sediment Subcompartment Volumes, m^3

Solids	103
Pore-Water	581

	Density kg/m^3	Concentration of Particles	Volume Fraction	OC Fraction
Particles In Water Column	2400	100 mg/L	4.17E-05	0.24
Sediment Solids	2400		0.1500	0.04
Inflow Particles	2400	100 mg/L	4.17E-05	0.24
Resuspended Particles	2400			0.035
Aerosols In Air	1500	41.75 µg/m^3	2.78E-11	

Mass Transfer Coefficients	m/h
Volatilization (air side)	1.00
Volatilization (water side)	0.0100
Sediment-water Diffusion	4.00E-04
Aerosol Dry Deposition Velocity	7.20
Aerosol Scavenging Ratio	2.00E+05

	m^3/h	
Rain Rate	4.74	2.43 m/year
Sediment Deposition	5.09E-04	1.72 g/m^2day
Sediment Resuspension	1.78E-04	0.6000 g/m^2day
Sediment Burial	1.48E-04	0.5000 g/m^2day

Aerosol Deposition Rate	m^3/h
Wet	2.64E-05
Dry	3.43E-06
Total	2.98E-05

Chrysene (Results) of Sampling Point S3

Amounts

	mol	kg	%
Bulk Water	0.0694	0.0158	27.51
Water Solution	9.82E-03	2.24E-03	3.89
Water Particles	0.0596	0.0136	23.62
Bulk Sediment	0.1828	0.0417	72.49
Sediment Pore Water	4.27E-05	9.74E-06	0.0169
Sediment Solids	0.1828	0.0417	72.47
System Total	0.2522	0.0576	2824

Amount Sorbed
(% of amount in bulk phase)

	%
Water	85.85
Sediment	99.98
Inflow	85.85
Air	1.07

Emission	0	kg/year
Chemical Concentration in Inflow	1670	ng/L
Chemical Concentration in Air	0	ng/m³

	D Value mol/Pa.h	Response Time of Water years	Response Time of Sediment years
Burial	0.3363		78.92
Sediment Transformation	18.39		1.44
Sediment Resuspension	0.3531	10.94	75.16
Water To Sediment Diffusion	0.6385	6.05	41.57
Sediment Deposition	6.92	0.5579	3.83
Water Transformation	2606	1.48E-03	
Volatilization	4.82	0.8020	
Volat. (air side)	6.90		
Volat. (water side)	15.96		
Water Outflow	84.01	0.0460	
Water Particle Outflow	510	7.58E-03	
Rain Dissolution	0.4422	8.74	
Wet Particle Deposition	4.13	0.9356	
Dry Particle Deposition	0.5365	7.20	
Water Inflow	84.01	0.0460	
Water Particle Inflow	510	7.58E-03	

- (•) years
- ( ) days
- ( ) hours

	Fugacity	Z Values	Concentrations			
	Pa	mol/m³Pa	kg/m³			mol/(m³ of bulk)
Bulk Air	0	4.08E-04	0	0	ng/m³	
Air vapour		4.03E-04	0			
Aerosols		1.57E+05	0			0
Bulk Water	2.05E-06	0.6597	3.09E-07	309	ng/L	
Water Solution		0.0933	4.37E-08			
Water Particles		13592	6.36E-03	2651	ng/g	1.16E-06
Bulk Inflow	1.11E-05	0.6597	1.67E-06	1670	ng/L	
Inflow Water			2.36E-07			
Inflow Particles		13592	0.0344			6.28E-06
Bulk Sediment	7.86E-07	340	6.10E-05	6.10E+07	ng/m³	
Sediment Pore Water			1.68E-08	16.75	ng/L	
Sediment Solids		2265	4.07E-04	169	ng/g	2.67E-04
Resuspended Solids		1982				
Rain	0		0	0	ng/L	

(•) kg/m³
( ) mol/m³

In the System

	mol/h	kg/year
Total Chemical Inputs	6.58E-03	13.17
Emission	0	0
Inflow	6.58E-03	13.17
Air to water transfer	0	0
Total Chemical Losses	6.58E-03	13.17
Outflow	1.22E-03	2.43
Water to air transfer	9.87E-06	0.0197
Total Transformation	5.36E-03	10.71
Sediment Burial	2.64E-07	5.29E-04

(•) System
( ) Water
( ) Sediment

Residence Time (not including water-sediment exchange as a loss)

Water	10.56 h	0.4400 d	1.21E-03 y
Sediment	12414 h	517 d	1.42 y
System	38.30 h	1.60 d	4.37E-03 y

Emission to Water	0	Water to Sediment Diffusion	2.62E-03
Water Inflow	1.86	Sediment to Water Diffusion	1.00E-03
Particle Inflow	11.30		
		Water Transformation	10.68
Rain Dissolution	0	Sediment Transformation	0.0289
Aerosol Deposition - Wet	0		
Aerosol Deposition - Dry	0	Sediment Burial	5.29E-04
Absorption	0	Water Outflow	0.3444
Volatilization	0.0197	Particle Outflow	2.09
Sediment Deposition	0.0284		
Sediment Resuspension	5.55E-04		

(•) kg/year
( ) mol/h

APPENDIX 8

QWASI 3.10 INPUT AND FULL RESULTS

Dibenz(a,h)anthracene from S1,2,S3, and S4

Dibenz(a,h)anthracene (Chemical Parameters) of Sampling Point S1

	Half-Life	Rate Constant
	h	1/h
Water	6.00	0.1155
Sediment	15612	4.44E-05

		L/kg
Air-Water (Kaw)	6.29E-07	-
Suspended Particles-Water	1.33E+06	5.53E+05
Sediment-Water	2.21E+05	92224
Resuspended Particles-Water	1.94E+05	80696
Aerosol-Air	8.86E+12	-
Organic Carbon-Water (Koc)	-	2.31E+06

Chemical Type	1			
Molar Mass	278	g/mol		
Temperature	25.00	°C	298	K
Log Kow	6.75			
Solubility	5.00E-04	g/m³	1.80E-06	mol/m³
Vapour Pressure	2.80E-09	Pa		
Melting Point	266	°C	539	K
Sub-cooled Liquid				
Vapour Pressure	6.77E-07	Pa		
Fugacity Ratio	4.13E-03			
Henry's Law Constant	1.56E-03	Pa.m³/mol		

Dibenz(a,h)anthracene(Environmental Parameters) of Sampling Point S1

	Area	Depth	Volume
	m^2	m	m^3
Water	17100	3.00	51300
Sediment	17100	0.0400	684

	Inflow	Outflow
Water	900m^3/h	900m^3/h
Suspended Particles	0.0375m^3/h	0.0375m^3/h

Sediment Subcompartment Volumes, m^3

Solids	103
Pore-Water	581

	Density	Concentration	Volume	OC
	kg/m^3	of Particles	Fraction	Fraction
Particles In Water Column	2400	100 mg/L	4.17E-05	0.24
Sediment Solids	2400		0.1500	0.04
Inflow Particles	2400	100 mg/L	4.17E-05	0.24
Resuspended Particles	2400			0.035
Aerosols In Air	1500	41.75 µg/m^3	2.78E-11	

Mass Transfer Coefficients	m/h
Volatilization (air side)	1.00
Volatilization (water side)	0.0100
Sediment-water Diffusion	4.00E-04
Aerosol Dry Deposition Velocity	7.20
Aerosol Scavenging Ratio	2.00E+05

	m^3/h	
Rain Rate	4.74	2.43 m/year
Sediment Deposition	5.09E-04	1.72 g/m^2day
Sediment Resuspension	1.78E-04	0.6000 g/m^2day
Sediment Burial	1.48E-04	0.5000 g/m^2day

Aerosol Deposition Rate	m^3/h
Wet	2.64E-05
Dry	3.43E-06
Total	2.98E-05

Dibenz(a,h)anthracene (Results) of Sampling Point S1

Amounts

	mol	kg	%
Bulk Water	0.3470	0.0966	16.77
Water Solution	6.16E-03	1.71E-03	0.2977
Water Particles	0.3408	0.0949	16.48
Bulk Sediment	1.72	0.4792	83.23
Sediment Pore Water	4.41E-05	1.23E-05	2.13E-03
Sediment Solids	1.72	0.4792	83.23
System Total	2.07	0.5758	1761

Amount Sorbed
(% of amount in bulk phase)

	%
Water	98.22
Sediment	100.00
Inflow	98.23
Air	99.60

Emission	0	kg/year
Chemical Concentration in Inflow	14300	ng/L
Chemical Concentration in Air	0	ng/m³

	D Value mol/Pa.h	Response Time of Water years	Response Time of Sediment years
Burial	21078		78.91
Sediment Transformation	6.47E+05		2.57
Sediment Resuspension	22132	9.56	75.15
Water To Sediment Diffusion	4388	48.23	379
Sediment Deposition	4.34E+05	0.4876	3.83
Water Transformation	2.14E+08	9.88E-04	
Volatilization	6.90	30682	
Volat. (air side)	6.90		
Volat. (water side)	1.10E+05		
Water Outflow	5.77E+05	0.3666	
Water Particle Outflow	3.19E+07	6.62E-03	
Rain Dissolution	3039	69.63	
Wet Particle Deposition	94252	2.25	
Dry Particle Deposition	12247	17.28	
Water Inflow	5.77E+05	0.3666	
Water Particle Inflow	3.19E+07	6.62E-03	

(•) years
( ) days
( ) hours

	Fugacity	Z Values	Concentrations			
	Pa	mol/m³Pa	kg/m³			mol/(m³ of bulk)
Bulk Air	0	0.0999	0	0	ng/m³	
Air vapour		4.03E-04	0			
Aerosols		3.57E+09	0			0
Bulk Water	1.87E-10	36141	1.88E-06	1883	ng/L	
Water Solution		642	3.34E-08			
Water Particles		8.52E+08	0.0444	18491	ng/g	6.64E-06
Bulk Inflow	1.42E-09	36139	1.43E-05	14300	ng/L	
Inflow Water			2.54E-07			
Inflow Particles		8.52E+08	0.3371			5.05E-05
Bulk Sediment	1.18E-10	2.13E+07	7.01E-04	7.01E+08	ng/m³	
Sediment Pore Water			2.11E-08	21.10	ng/L	
Sediment Solids		1.42E+08	4.67E-03	1946	ng/g	2.52E-03
Resuspended Solids		1.24E+08				
Rain	0		0	0	ng/L	

kg/m³
mol/m³

In the System

	mol/h	kg/year		
Total Chemical Inputs	0.0462	113		
Emission	0	0		
Inflow	0.0462	113		
Air to water transfer	0	0		
Total Chemical Losses	0.0462	113		
Outflow	6.09E-03	14.84		
Water to air transfer	1.29E-09	3.15E-06		
Total Transformation	0.0401	97.90		
Sediment Burial	2.49E-06	6.07E-03		
Residence Time (not including water-sediment exchange as a loss)				
Water	7.52 h	0.3132 d	8.58E-04 y	
Sediment	21817 h	909 d	2.49 y	
System	44.74 h	1.86 d	5.11E-03 y	

System
Water
Sediment

Emission to Water	0	Water to Sediment Diffusion	2.00E-03
Water Inflow	2.00	Sediment to Water Diffusion	1.26E-03
Particle Inflow	111		
		Water Transformation	97.71
Rain Dissolution	0	Sediment Transformation	0.1863
Aerosol Deposition - Wet	0		
Aerosol Deposition - Dry	0	Sediment Burial	6.07E-03
Absorption	0	Water Outflow	0.2635
Volatilization	3.15E-06	Particle Outflow	14.58
Sediment Deposition	0.1980		
Sediment Resuspension	6.38E-03		

kg/year
mol/h

Dibenz(a,h)anthracene (Chemical Parameters) of Sampling Point S2

	Half-Life	Rate Constant
	h	1/h
Water	6.00	0.1155
Sediment	15612	4.44E-05

		L/kg
Air-Water (Kaw)	6.29E-07	-
Suspended Particles-Water	1.33E+06	5.53E+05
Sediment-Water	2.21E+05	92224
Resuspended Particles-Water	1.94E+05	80696
Aerosol-Air	8.86E+12	-
Organic Carbon-Water (Koc)	-	2.31E+06

Chemical Type	1			
Molar Mass	278	g/mol		
Temperature	25.00	°C	298	K
Log Kow	6.75			
Solubility	5.00E-04	g/m³	1.80E-06	mol/m³
Vapour Pressure	2.80E-09	Pa		
Melting Point	266	°C	539	K
Sub-cooled Liquid				
Vapour Pressure	6.77E-07	Pa		
Fugacity Ratio	4.13E-03			
Henry's Law Constant	1.56E-03	Pa.m³/mol		

Dibenz(a,h)anthracene(Environmental Parameters) of Sampling Point S2

	Area	Depth	Volume
	m^2	m	m^3
Water	17100	3.00	51300
Sediment	17100	0.0400	684

	Inflow	Outflow
Water	900m^3/h	900m^3/h
Suspended Particles	0.0375m^3/h	0.0375m^3/h

Sediment Subcompartment Volumes, m^3

Solids	103
Pore-Water	581

	Density kg/m^3	Concentration of Particles	Volume Fraction	OC Fraction
Particles In Water Column	2400	100 mg/L	4.17E-05	0.24
Sediment Solids	2400		0.1500	0.04
Inflow Particles	2400	100 mg/L	4.17E-05	0.24
Resuspended Particles	2400			0.035
Aerosols In Air	1500	41.75 µg/m^3	2.78E-11	

Mass Transfer Coefficients	m/h
Volatilization (air side)	1.00
Volatilization (water side)	0.0100
Sediment-water Diffusion	4.00E-04
Aerosol Dry Deposition Velocity	7.20
Aerosol Scavenging Ratio	2.00E+05

	m^3/h	
Rain Rate	4.74	2.43 m/year
Sediment Deposition	5.09E-04	1.72 g/m^2day
Sediment Resuspension	1.78E-04	0.6000 g/m^2day
Sediment Burial	1.48E-04	0.5000 g/m^2day

Aerosol Deposition Rate	m^3/h
Wet	2.64E-05
Dry	3.43E-06
Total	2.98E-05

Dibenz(a,h)anthracene (Results) of Sampling Point S2

Amounts

	mol	kg	%
Bulk Water	0.3089	0.0860	16.77
Water Solution	5.48E-03	1.53E-03	0.2977
Water Particles	0.3034	0.0844	16.48
Bulk Sediment	1.53	0.4266	83.23
Sediment Pore Water	3.92E-05	1.09E-05	2.13E-03
Sediment Solids	1.53	0.4266	83.23
System Total	1.84	0.5126	1761

Amount Sorbed
(% of amount in bulk phase)

	%
Water	98.22
Sediment	100.00
Inflow	98.23
Air	99.60

Emission	0	kg/year
Chemical Concentration in Inflow	12730	ng/L
Chemical Concentration in Air	0	ng/m³

	D Value mol/Pa.h	Response Time of Water years	Response Time of Sediment years
Burial	21078		78.91
Sediment Transformation	6.47E+05		2.57
Sediment Resuspension	22132	9.56	75.15
Water To Sediment Diffusion	4388	48.23	379
Sediment Deposition	4.34E+05	0.4876	3.83
Water Transformation	2.14E+08	9.88E-04	
Volatilization	6.90	30682	
Volat. (air side)	6.90		
Volat. (water side)	1.10E+05		
Water Outflow	5.77E+05	0.3666	
Water Particle Outflow	3.19E+07	6.62E-03	
Rain Dissolution	3039	69.63	
Wet Particle Deposition	94252	2.25	
Dry Particle Deposition	12247	17.28	
Water Inflow	5.77E+05	0.3666	
Water Particle Inflow	3.19E+07	6.62E-03	

(•) years
( ) days
( ) hours

	Fugacity	Z Values	Concentrations			
	Pa	mol/m^{3}Pa	kg/m^3			mol/(m^3 of bulk)
Bulk Air	0	0.0999	0	0	ng/m^3	
Air vapour		4.03E-04	0			
Aerosols		3.57E+09	0			0
Bulk Water	1.67E-10	36141	1.68E-06	1676	ng/L	
Water Solution		642	2.97E-08			
Water Particles		8.52E+08	0.0395	16461	ng/g	5.91E-06
Bulk Inflow	1.27E-09	36139	1.27E-05	12730	ng/L	
Inflow Water			2.26E-07			
Inflow Particles		8.52E+08	0.3001			4.49E-05
Bulk Sediment	1.05E-10	2.13E+07	6.24E-04	6.24E+08	ng/m^3	
Sediment Pore Water			1.88E-08	18.78	ng/L	
Sediment Solids		1.42E+08	4.16E-03	1732	ng/g	2.24E-03
Resuspended Solids		1.24E+08				
Rain	0		0	0	ng/L	

(•) kg/m^3
( ) mol/m^3

In the System

	mol/h	kg/year
Total Chemical Inputs	0.0412	100
Emission	0	0
Inflow	0.0412	100
Air to water transfer	0	0
Total Chemical Losses	0.0412	100
Outflow	5.42E-03	13.21
Water to air transfer	1.15E-09	2.80E-06
Total Transformation	0.0357	87.15
Sediment Burial	2.22E-06	5.41E-03

(•) System
( ) Water
( ) Sediment

Residence Time (not including water-sediment exchange as a loss)

Water	7.52 h	0.3132 d	8.58E-04 y
Sediment	21817 h	909 d	2.49 y
System	44.74 h	1.86 d	5.11E-03 y

Emission to Water	0	Water to Sediment Diffusion	1.78E-03
Water Inflow	1.78	Sediment to Water Diffusion	1.13E-03
Particle Inflow	98.59		
		Water Transformation	86.98
Rain Dissolution	0	Sediment Transformation	0.1659
Aerosol Deposition - Wet	0		
Aerosol Deposition - Dry	0	Sediment Burial	5.41E-03
Absorption	0	Water Outflow	0.2345
Volatilization	2.80E-06	Particle Outflow	12.98
Sediment Deposition	0.1763		
Sediment Resuspension	5.68E-03		

(•) kg/year
( ) mol/h

Dibenz(a,h)anthracene (Chemical Parameters) of Sampling Point S3

	Half-Life h	Rate Constant 1/h
Water	6.00	0.1155
Sediment	15612	4.44E-05

		L/kg
Air-Water (Kaw)	6.29E-07	-
Suspended Particles-Water	1.33E+06	5.53E+05
Sediment-Water	2.21E+05	92224
Resuspended Particles-Water	1.94E+05	80696
Aerosol-Air	8.86E+12	-
Organic Carbon-Water (Koc)	-	2.31E+06

Chemical Type	1			
Molar Mass	278	g/mol		
Temperature	25.00	°C	298	K
Log Kow	6.75			
Solubility	5.00E-04	g/m³	1.80E-06	mol/m³
Vapour Pressure	2.80E-09	Pa		
Melting Point	266	°C	539	K
Sub-cooled Liquid				
Vapour Pressure	6.77E-07	Pa		
Fugacity Ratio	4.13E-03			
Henry's Law Constant	1.56E-03	Pa.m³/mol		

Dibenz(a,h)anthracene(Environmental Parameters) of Sampling Point S3

	Area	Depth	Volume
	m^2	m	m^3
Water	17100	3.00	51300
Sediment	17100	0.0400	684

	Inflow	Outflow
Water	900m^3/h	900m^3/h
Suspended Particles	0.0375m^3/h	0.0375m^3/h

Sediment Subcompartment Volumes, m^3

Solids	103
Pore-Water	581

	Density kg/m^3	Concentration of Particles	Volume Fraction	OC Fraction
Particles In Water Column	2400	100 mg/L	4.17E-05	0.24
Sediment Solids	2400		0.1500	0.04
Inflow Particles	2400	100 mg/L	4.17E-05	0.24
Resuspended Particles	2400			0.035
Aerosols In Air	1500	41.75 µg/m^3	2.78E-11	

Mass Transfer Coefficients	m/h
Volatilization (air side)	1.00
Volatilization (water side)	0.0100
Sediment-water Diffusion	4.00E-04
Aerosol Dry Deposition Velocity	7.20
Aerosol Scavenging Ratio	2.00E+05

	m^3/h	
Rain Rate	4.74	2.43 m/year
Sediment Deposition	5.09E-04	1.72 g/m^2day
Sediment Resuspension	1.78E-04	0.6000 g/m^2day
Sediment Burial	1.48E-04	0.5000 g/m^2day

Aerosol Deposition Rate	m^3/h
Wet	2.64E-05
Dry	3.43E-06
Total	2.98E-05

Dibenz(a,h)anthracene (Results) of Sampling Point S3

Amounts

	mol	kg	%
Bulk Water	1.04	0.2909	16.77
Water Solution	0.0185	5.16E-03	0.2977
Water Particles	1.03	0.2857	16.48
Bulk Sediment	5.19	1.44	83.23
Sediment Pore Water	1.33E-04	3.70E-05	2.13E-03
Sediment Solids	5.19	1.44	83.23
System Total	6.23	1.73	1761

Amount Sorbed
(% of amount in bulk phase)

	%
Water	98.22
Sediment	100.00
Inflow	98.23
Air	99.60

Emission	0	kg/year
Chemical Concentration in Inflow	43070	ng/L
Chemical Concentration in Air	0	ng/m³

	D Value mol/Pa.h	Response Time of Water years	Response Time of Sediment years
Burial	21078		78.91
Sediment Transformation	6.47E+05		2.57
Sediment Resuspension	22132	9.56	75.15
Water To Sediment Diffusion	4388	48.23	379
Sediment Deposition	4.34E+05	0.4876	3.83
Water Transformation	2.14E+08	9.88E-04	
Volatilization	6.90	30682	
Volat. (air side)	6.90		
Volat. (water side)	1.10E+05		
Water Outflow	5.77E+05	0.3666	
Water Particle Outflow	3.19E+07	6.62E-03	
Rain Dissolution	3039	69.63	
Wet Particle Deposition	94252	2.25	
Dry Particle Deposition	12247	17.28	
Water Inflow	5.77E+05	0.3666	
Water Particle Inflow	3.19E+07	6.62E-03	

(•) years
( ) days
( ) hours

	Fugacity	Z Values	Concentrations			
	Pa	mol/m³Pa	kg/m³			mol/(m³ of bulk)
Bulk Air	0	0.0999	0	0	ng/m³	
Air vapour		4.03E-04	0			
Aerosols		3.57E+09	0			0
Bulk Water	5.64E-10	36141	5.67E-06	5670	ng/L	
Water Solution		642	1.01E-07			
Water Particles		8.52E+08	0.1337	55693	ng/g	2.00E-05
Bulk Inflow	4.28E-09	36139	4.31E-05	43070	ng/L	
Inflow Water			7.65E-07			
Inflow Particles		8.52E+08	1.02			1.52E-04
Bulk Sediment	3.56E-10	2.13E+07	2.11E-03	2.11E+09	ng/m³	
Sediment Pore Water			6.36E-08	63.55	ng/L	
Sediment Solids		1.42E+08	0.0141	5861	ng/g	7.58E-03
Resuspended Solids		1.24E+08				
Rain	0		0	0	ng/L	

kg/m³
mol/m³

In the System

	mol/h	kg/year
Total Chemical Inputs	0.1393	340
Emission	0	0
Inflow	0.1393	340
Air to water transfer	0	0
Total Chemical Losses	0.1393	340
Outflow	0.0183	44.70
Water to air transfer	3.89E-09	9.48E-06
Total Transformation	0.1209	295
Sediment Burial	7.50E-06	0.0183

System
Water
Sediment

Residence Time (not including water-sediment exchange as a loss)

Water	7.52 h	0.3132 d	8.58E-04 y
Sediment	21817 h	909 d	2.49 y
System	44.74 h	1.86 d	5.11E-03 y

Emission to Water	0	Water to Sediment Diffusion	6.03E-03
Water Inflow	6.03	Sediment to Water Diffusion	3.81E-03
Particle Inflow	334		
		Water Transformation	294
Rain Dissolution	0	Sediment Transformation	0.5612
Aerosol Deposition - Wet	0		
Aerosol Deposition - Dry	0	Sediment Burial	0.0183
Absorption	0	Water Outflow	0.7935
Volatilization	9.48E-06	Particle Outflow	43.91
Sediment Deposition	0.5965		
Sediment Resuspension	0.0192		

kg/year
mol/h

Dibenz(a,h)anthracene (Chemical Parameters) of Sampling Point S4

	Half-Life	Rate Constant
	h	1/h
Water	6.00	0.1155
Sediment	15612	4.44E-05

		L/kg
Air-Water (Kaw)	6.29E-07	-
Suspended Particles-Water	1.33E+06	5.53E+05
Sediment-Water	2.21E+05	92224
Resuspended Particles-Water	1.94E+05	80696
Aerosol-Air	8.86E+12	-
Organic Carbon-Water (Koc)	-	2.31E+06

Chemical Type	1			
Molar Mass	278	g/mol		
Temperature	25.00	°C	298	K
Log Kow	6.75			
Solubility	5.00E-04	g/m³	1.80E-06	mol/m³
Vapour Pressure	2.80E-09	Pa		
Melting Point	266	°C	539	K
Sub-cooled Liquid				
Vapour Pressure	6.77E-07	Pa		
Fugacity Ratio	4.13E-03			
Henry's Law Constant	1.56E-03	Pa.m³/mol		

Dibenz(a,h)anthracene(Environmental Parameters) of Sampling Point S4

	Area	Depth	Volume
	m^2	m	m^3
Water	17100	3.00	51300
Sediment	17100	0.0400	684

	Inflow	Outflow
Water	900m^3/h	900m^3/h
Suspended Particles	0.0375m^3/h	0.0375m^3/h

Sediment Subcompartment Volumes, m^3

Solids	103
Pore-Water	581

	Density kg/m^3	Concentration of Particles	Volume Fraction	OC Fraction
Particles In Water Column	2400	100 mg/L	4.17E-05	0.24
Sediment Solids	2400		0.1500	0.04
Inflow Particles	2400	100 mg/L	4.17E-05	0.24
Resuspended Particles	2400			0.035
Aerosols In Air	1500	41.75 µg/m^3	2.78E-11	

Mass Transfer Coefficients	m/h
Volatilization (air side)	1.00
Volatilization (water side)	0.0100
Sediment-water Diffusion	4.00E-04
Aerosol Dry Deposition Velocity	7.20
Aerosol Scavenging Ratio	2.00E+05

	m^3/h	
Rain Rate	4.74	2.43 m/year
Sediment Deposition	5.09E-04	1.72 g/m^2day
Sediment Resuspension	1.78E-04	0.6000 g/m^2day
Sediment Burial	1.48E-04	0.5000 g/m^2day

Aerosol Deposition Rate	m^3/h
Wet	2.64E-05
Dry	3.43E-06
Total	2.98E-05

Dibenz(a,h)anthracene (Results) of Sampling Point S4

Amounts

	mol	kg	%
Bulk Water	0.0934	0.0260	16.77
Water Solution	1.66E-03	4.62E-04	0.2977
Water Particles	0.0918	0.0255	16.48
Bulk Sediment	0.4635	0.1290	83.23
Sediment Pore Water	1.19E-05	3.30E-06	2.13E-03
Sediment Solids	0.4635	0.1290	83.23
System Total	0.5569	0.1550	1761

Amount Sorbed
(% of amount in bulk phase)

	%
Water	98.22
Sediment	100.00
Inflow	98.23
Air	99.60

Emission	0	kg/year
Chemical Concentration in Inflow	3850	ng/L
Chemical Concentration in Air	0	ng/m³

	D Value mol/Pa.h	Response Time of Water years	Response Time of Sediment years
Burial	21078		78.91
Sediment Transformation	6.47E+05		2.57
Sediment Resuspension	22132	9.56	75.15
Water To Sediment Diffusion	4388	48.23	379
Sediment Deposition	4.34E+05	0.4876	3.83
Water Transformation	2.14E+08	9.88E-04	
Volatilization	6.90	30682	
Volat. (air side)	6.90		
Volat. (water side)	1.10E+05		
Water Outflow	5.77E+05	0.3666	
Water Particle Outflow	3.19E+07	6.62E-03	
Rain Dissolution	3039	69.63	
Wet Particle Deposition	94252	2.25	
Dry Particle Deposition	12247	17.28	
Water Inflow	5.77E+05	0.3666	
Water Particle Inflow	3.19E+07	6.62E-03	

(•) years
( ) days
( ) hours

	Fugacity	Z Values	Concentrations			
	Pa	mol/m³Pa	kg/m³			mol/(m³ of bulk)
Bulk Air	0	0.0999	0	0	ng/m³	
Air vapour		4.03E-04	0			
Aerosols		3.57E+09	0			0
Bulk Water	5.04E-11	36141	5.07E-07	507	ng/L	
Water Solution		642	9.00E-09			
Water Particles		8.52E+08	0.0119	4978	ng/g	1.79E-06
Bulk Inflow	3.83E-10	36139	3.85E-06	3850	ng/L	
Inflow Water			6.83E-08			
Inflow Particles		8.52E+08	0.0908			1.36E-05
Bulk Sediment	3.18E-11	2.13E+07	1.89E-04	1.89E+08	ng/m³	
Sediment Pore Water			5.68E-09	5.68	ng/L	
Sediment Solids		1.42E+08	1.26E-03	524	ng/g	6.78E-04
Resuspended Solids		1.24E+08				
Rain	0		0	0	ng/L	

(•) kg/m³
( ) mol/m³

In the System

	mol/h	kg/year
Total Chemical Inputs	0.0124	30.35
Emission	0	0
Inflow	0.0124	30.35
Air to water transfer	0	0
Total Chemical Losses	0.0124	30.35
Outflow	1.64E-03	4.00
Water to air transfer	3.48E-10	8.47E-07
Total Transformation	0.0108	26.36
Sediment Burial	6.71E-07	1.64E-03

(•) System
( ) Water
( ) Sediment

Residence Time (not including water-sediment exchange as a loss)

Water	7.52 h	0.3132 d	8.58E-04 y
Sediment	21817 h	909 d	2.49 y
System	44.74 h	1.86 d	5.11E-03 y

Emission to Water	0	Water to Sediment Diffusion	5.39E-04
Water Inflow	0.5388	Sediment to Water Diffusion	3.40E-04
Particle Inflow	29.82		
		Water Transformation	26.31
Rain Dissolution	0	Sediment Transformation	0.0502
Aerosol Deposition - Wet	0		
Aerosol Deposition - Dry	0	Sediment Burial	1.64E-03
Absorption	0	Water Outflow	0.0709
Volatilization	8.47E-07	Particle Outflow	3.92
Sediment Deposition	0.0533		
Sediment Resuspension	1.72E-03		

(•) kg/year
( ) mol/h

APPENDIX 9

QWASI 3.10 INPUT AND FULL RESULTS

Indeno(1,2,3-cd)pyrene from S1 and S3

Indeno(1,2,3-cd)pyrene (Chemical Parameters) of Sampling Point S1

	Half-Life	Rate Constant
	h	1/h
Water	9.50	0.0729
Sediment	9360	7.40E-05

		L/kg
Air-Water (Kaw)	5.87E-04	-
Suspended Particles-Water	1.05E+06	4.40E+05
Sediment-Water	1.76E+05	73256
Resuspended Particles-Water	1.54E+05	64099
Aerosol-Air	2.55E+11	-
Organic Carbon-Water (Koc)	-	1.83E+06

Chemical Type	1			
Molar Mass	276	g/mol		
Temperature	25.00	°C	298	K
Log Kow	6.65			
Solubility	1.90E-04	g/m³	6.88E-07	mol/m³
Vapour Pressure	1.00E-06	Pa		
Melting Point	164	°C	437	K
Sub-cooled Liquid				
Vapour Pressure	2.35E-05	Pa		
Fugacity Ratio	0.0426			
Henry's Law Constant	1.45	Pa.m³/mol		

Indeno(1,2,3-cd)pyrene (Environmental Parameters) Sampling Point S1

	Area	Depth	Volume
	m^2	m	m^3
Water	17100	3.00	51300
Sediment	17100	0.0400	684

	Inflow	Outflow
Water	900m^3/h	900m^3/h
Suspended Particles	0.0375m^3/h	0.0375m^3/h

Sediment Subcompartment Volumes, m^3

Solids	103
Pore-Water	581

	Density	Concentration	Volume	OC
	kg/m^3	of Particles	Fraction	Fraction
Particles In Water Column	2400	100 mg/L	4.17E-05	0.24
Sediment Solids	2400		0.1500	0.04
Inflow Particles	2400	100 mg/L	4.17E-05	0.24
Resuspended Particles	2400			0.035
Aerosols In Air	1500	41.75 µg/m^3	2.78E-11	

Mass Transfer Coefficients	m/h
Volatilization (air side)	1.00
Volatilization (water side)	0.0100
Sediment-water Diffusion	4.00E-04
Aerosol Dry Deposition Velocity	7.20
Aerosol Scavenging Ratio	2.00E+05

	m^3/h	
Rain Rate	4.74	2.43 m/year
Sediment Deposition	5.09E-04	1.72 g/m^2day
Sediment Resuspension	1.78E-04	0.6000 g/m^2day
Sediment Burial	1.48E-04	0.5000 g/m^2day

Aerosol Deposition Rate	m^3/h
Wet	2.64E-05
Dry	3.43E-06
Total	2.98E-05

Indeno(1,2,3-cd)pyrene (Results) of Sampling Point S1

Amounts

	mol	kg	%
Bulk Water	0.1407	0.0389	24.69
Water Solution	3.13E-03	8.65E-04	0.5493
Water Particles	0.1376	0.0380	24.14
Bulk Sediment	0.4292	0.1186	75.31
Sediment Pore Water	1.38E-05	3.82E-06	2.43E-03
Sediment Solids	0.4292	0.1186	75.30
System Total	0.5699	0.1575	2545

Amount Sorbed
(% of amount in bulk phase)

	%
Water	97.78
Sediment	100.00
Inflow	97.78
Air	87.67

Emission	0	kg/year
Chemical Concentration in Inflow	3920	ng/L
Chemical Concentration in Air	0	ng/m³

	D Value mol/Pa.h	Response Time of Water years	Response Time of Sediment years
Burial	17.94		78.91
Sediment Transformation	918		1.54
Sediment Resuspension	18.84	9.61	75.15
Water To Sediment Diffusion	4.70	38.49	301
Sediment Deposition	370	0.4899	3.83
Water Transformation	1.16E+05	1.56E-03	
Volatilization	6.52	27.78	
Volat. (air side)	6.90		
Volat. (water side)	118		
Water Outflow	619	0.2925	
Water Particle Outflow	27200	6.65E-03	
Rain Dissolution	3.26	55.57	
Wet Particle Deposition	2718	0.0666	
Dry Particle Deposition	353	0.5125	
Water Inflow	619	0.2925	
Water Particle Inflow	27200	6.65E-03	

(•) years
( ) days
( ) hours

	Fugacity	Z Values	Concentrations			
	Pa	mol/m³Pa	kg/m³			mol/(m³ of bulk)
Bulk Air	0	3.27E-03	0	0	ng/m³	
Air vapour		4.03E-04	0			
Aerosols		1.03E+08	0			0
Bulk Water	8.88E-08	30.91	7.58E-07	758	ng/L	
Water Solution		0.6876	1.69E-08			
Water Particles		7.25E+05	0.0178	7412	ng/g	2.68E-06
Bulk Inflow	4.59E-07	30.91	3.92E-06	3920	ng/L	
Inflow Water			8.72E-08			
Inflow Particles		7.25E+05	0.0920			1.39E-05
Bulk Sediment	3.46E-08	18134	1.73E-04	1.73E+08	ng/m³	
Sediment Pore Water			6.57E-09	6.57	ng/L	
Sediment Solids		1.21E+05	1.16E-03	482	ng/g	6.27E-04
Resuspended Solids		1.06E+05				
Rain	0		0	0	ng/L	

(•) kg/m³
( ) mol/m³

In the System

	mol/h	kg/year
Total Chemical Inputs	0.0128	30.91
Emission	0	0
Inflow	0.0128	30.91
Air to water transfer	0	0
Total Chemical Losses	0.0128	30.91
Outflow	2.47E-03	5.98
Water to air transfer	5.78E-07	1.40E-03
Total Transformation	0.0103	24.93
Sediment Burial	6.21E-07	1.50E-03

(•) System
( ) Water
( ) Sediment

Residence Time (not including water-sediment exchange as a loss)

Water	11.05 h	0.4604 d	1.26E-03 y
Sediment	13248 h	552 d	1.51 y
System	44.64 h	1.86 d	5.10E-03 y

Emission to Water	0	Water to Sediment Diffusion	1.01E-03
Water Inflow	0.6875	Sediment to Water Diffusion	3.94E-04
Particle Inflow	30.22		
		Water Transformation	24.85
Rain Dissolution	0	Sediment Transformation	0.0769
Aerosol Deposition - Wet	0		
Aerosol Deposition - Dry	0	Sediment Burial	1.50E-03
Absorption	0	Water Outflow	0.1329
Volatilization	1.40E-03	Particle Outflow	5.84
Sediment Deposition	0.0794		
Sediment Resuspension	1.58E-03		

(•) kg/year
( ) mol/h

Indeno(1,2,3-cd)pyrene (Chemical Parameters) of Sampling Point S3

	Half-Life	Rate Constant
	h	1/h
Water	9.50	0.0729
Sediment	9360	7.40E-05

		L/kg
Air-Water (Kaw)	5.87E-04	-
Suspended Particles-Water	1.05E+06	4.40E+05
Sediment-Water	1.76E+05	73256
Resuspended Particles-Water	1.54E+05	64099
Aerosol-Air	2.55E+11	-
Organic Carbon-Water (Koc)	-	1.83E+06

Chemical Type	1			
Molar Mass	276	g/mol		
Temperature	25.00	°C	298	K
Log Kow	6.65			
Solubility	1.90E-04	g/m³	6.88E-07	mol/m³
Vapour Pressure	1.00E-06	Pa		
Melting Point	164	°C	437	K
Sub-cooled Liquid				
Vapour Pressure	2.35E-05	Pa		
Fugacity Ratio	0.0426			
Henry's Law Constant	1.45	Pa.m³/mol		

Indeno(1,2,3-cd)pyrene (Environmental Parameters) of Sampling Point S3

	Area	Depth	Volume
	m^2	m	m^3
Water	17100	3.00	51300
Sediment	17100	0.0400	684

	Inflow	Outflow
Water	900m^3/h	900m^3/h
Suspended Particles	0.0375m^3/h	0.0375m^3/h

Sediment Subcompartment Volumes, m^3

Solids	103
Pore-Water	581

	Density	Concentration	Volume	OC
	kg/m^3	of Particles	Fraction	Fraction
Particles In Water Column	2400	100 mg/L	4.17E-05	0.24
Sediment Solids	2400		0.1500	0.04
Inflow Particles	2400	100 mg/L	4.17E-05	0.24
Resuspended Particles	2400			0.035
Aerosols In Air	1500	41.75 µg/m^3	2.78E-11	

Mass Transfer Coefficients	m/h
Volatilization (air side)	1.00
Volatilization (water side)	0.0100
Sediment-water Diffusion	4.00E-04
Aerosol Dry Deposition Velocity	7.20
Aerosol Scavenging Ratio	2.00E+05

	m^3/h	
Rain Rate	4.74	2.43 m/year
Sediment Deposition	5.09E-04	1.72 g/m^2day
Sediment Resuspension	1.78E-04	0.6000 g/m^2day
Sediment Burial	1.48E-04	0.5000 g/m^2day

Aerosol Deposition Rate	m^3/h
Wet	2.64E-05
Dry	3.43E-06
Total	2.98E-05

Indeno(1,2,3-cd)pyrene (Results) of Sampling Point S3

Amounts

	mol	kg	%
Bulk Water	1.01	0.2778	24.69
Water Solution	0.0224	6.18E-03	0.5493
Water Particles	0.9829	0.2716	24.14
Bulk Sediment	3.07	0.8471	75.31
Sediment Pore Water	9.88E-05	2.73E-05	2.43E-03
Sediment Solids	3.07	0.8471	75.30
System Total	4.07	1.12	2545

Amount Sorbed
(% of amount in bulk phase)

	%
Water	97.78
Sediment	100.00
Inflow	97.78
Air	87.67

Emission	0	kg/year
Chemical Concentration in Inflow	28000	ng/L
Chemical Concentration in Air	0	ng/m³

	D Value mol/Pa.h	Response Time of Water years	Response Time of Sediment years
Burial	17.94		78.91
Sediment Transformation	918		1.54
Sediment Resuspension	18.84	9.61	75.15
Water To Sediment Diffusion	4.70	38.49	301
Sediment Deposition	370	0.4899	3.83
Water Transformation	1.16E+05	1.56E-03	
Volatilization	6.52	27.78	
Volat. (air side)	6.90		
Volat. (water side)	118		
Water Outflow	619	0.2925	
Water Particle Outflow	27200	6.65E-03	
Rain Dissolution	3.26	55.57	
Wet Particle Deposition	2718	0.0666	
Dry Particle Deposition	353	0.5125	
Water Inflow	619	0.2925	
Water Particle Inflow	27200	6.65E-03	

(•) years
( ) days
( ) hours

	Fugacity	Z Values	Concentrations			
	Pa	mol/m³Pa	kg/m³			mol/(m³ of bulk)
Bulk Air	0	3.27E-03	0	0	ng/m³	
Air vapour		4.03E-04	0			
Aerosols		1.03E+08	0			0
Bulk Water	6.34E-07	30.91	5.41E-06	5415	ng/L	
Water Solution		0.6876	1.20E-07			
Water Particles		7.25E+05	0.1271	52942	ng/g	1.92E-05
Bulk Inflow	3.28E-06	30.91	2.80E-05	28000	ng/L	
Inflow Water			6.23E-07			
Inflow Particles		7.25E+05	0.6571			9.91E-05
Bulk Sediment	2.47E-07	18134	1.24E-03	1.24E+09	ng/m³	
Sediment Pore Water			4.70E-08	46.96	ng/L	
Sediment Solids		1.21E+05	8.26E-03	3440	ng/g	4.48E-03
Resuspended Solids		1.06E+05				
Rain	0		0	0	ng/L	

(•) kg/m³
( ) mol/m³

In the System

	mol/h	kg/year
Total Chemical Inputs	0.0912	221
Emission	0	0
Inflow	0.0912	221
Air to water transfer	0	0
Total Chemical Losses	0.0912	221
Outflow	0.0176	42.69
Water to air transfer	4.13E-06	1.00E-02
Total Transformation	0.0736	178
Sediment Burial	4.44E-06	0.0107

(•) System
( ) Water
( ) Sediment

Residence Time (not including water-sediment exchange as a loss)

Water	11.05 h	0.4604 d	1.26E-03 y
Sediment	13248 h	552 d	1.51 y
System	44.64 h	1.86 d	5.10E-03 y

Emission to Water	0	Water to Sediment Diffusion	7.22E-03
Water Inflow	4.91	Sediment to Water Diffusion	2.81E-03
Particle Inflow	216		
		Water Transformation	178
Rain Dissolution	0	Sediment Transformation	0.5494
Aerosol Deposition - Wet	0		
Aerosol Deposition - Dry	0	Sediment Burial	0.0107
Absorption	0	Water Outflow	0.9496
Volatilization	1.00E-02	Particle Outflow	41.74
Sediment Deposition	0.5670		
Sediment Resuspension	0.0113		

(•) kg/year
( ) mol/h